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Identification of Organic Compounds in Industrial Effluent Discharges

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by

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FOREWORD

Nearly every phase of environmental protection depends on a capability to identify and measure specific pollutants in the environment. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Analytical Chemistry Branch identifies and measures chemical constituents of water and soil.

Concern has increased in recent years that man and his environment are being exposed to unknown industrial pollutants that may represent significant hazards. A basic step in assessing the problem is the identification and quantitation of compounds in industrial wastewaters that could appear in water supplies. The information in this report concerning organic compounds in industrial effluents will aid environmental decision-makers in assuring that human health and welfare are protected.

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Environmental Research Laboratory
Athens, Georgia

ABSTRACT

Samples of 63 effluent and 22 intake waters were collected from a wide range of chemical manufacturers in areas across the United States. The samples were analyzed for organic compounds in an effort to identify previously unknown and potentially hazardous organic pollutants. Each water sample was preconcentrated for analysis of organic compounds in four fractions: volatile organics by helium-gas stripping and semivolatile organics by extraction with methylene chloride resulting in separate neutral, acidic and basic fractions. All sample analyses involved a GC/MS/COMP system that used high-resolution glass capillary GC columns. Organic constituents were identified using the computerized Biemann mass spectral matching system together with some manual interpretation and quantified using GC-FID peak area determinations.

Over 570 compounds were tentatively identified of which 33 are priority pollutants. Generally, industrial effluents contained few priority pollutants. Most of the components found in the effluents were specific for a particular industrial site and did not appear in reoccurring patterns. The data suggest that many possible environmentally important compounds would be overlooked if frequency of occurrence is the major criterion for determining environmentally significant compounds.

We recommend that future studies concentrate on basic compound analyses and that the biological activity of a compound(s) be established first before exhaustive screening programs are initiated for environmental pollutants. Mass spectral data bases containing all the organic compounds produced by industry should be developed.

This report was submitted in fulfillment of Contract No. 68-01-4350 by Battelle, Columbus Laboratories, under the sponsorship of the U.S. Environmental Protection Agency. This report covers the period September 30, 1976, to November 30, 1978, and work was completed as of September 30, 1978.

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INTRODUCTION

There has been an increasing concern in recent years that man and his environment are being exposed to unknown industrial pollutants which may represent significant hazards. One approach to assessing the potential hazards involves a detailed chemical characterization of waste effluents. The objective of this program was the identification and quantification of organic compounds present in representative industrial final aqueous effluents. The information obtained will help the U.S. Environmental Protection Agency in its efforts in determining the health and environmental effects of industrial effluents, determining transport and degradation mechanisms, developing and assessing monitoring and control technology, and assessing wastewater disposal permits.

Priority was given to major industrial activities that were most apt to have significant amounts of organic compounds in their final aqueous effluents. Four different fractions from each effluent sample were analyzed by gas chromatography (GC) and gas chromatography-mass spectrometry (GC-MS) procedures. The fractions were acidic and neutral volatiles, neutral semivolatiles, acidic semivolatiles, and basic semivolatiles.

The program was designed as a cursory survey of wastewater effluent samples. A computerized mass spectral search system was used as the basis for compound identifications. High-resolution glass capillary GC columns were used to obtain the best possible mass spectra from the GC/MS/COMP systems. Because of the large number of samples, this program provided for only limited manual mass spectral interpretation.

CONCLUSIONS AND RECOMMENDATIONS

The conclusions and recommendations concerning this project are divided into three categories: (1) those which deal with the analytical protocol used in this program; (2) those which deal with the analytical results obtained; and (3) those concerned with the design of future studies for detecting environmentally significant pollutants.

ANALYTICAL PROTOCOL

- Stringent quality assurance protocols, such as those established for this program, must be followed during the performance of each analysis. Particularly important are instrument calibration (GC/MS/COMP), process and field blanks, uniformity of capillary GC system performance and recovery of representative standard compounds from spiked samples.
- Capillary column GC/MS for volatile analysis was demonstrated in this program to be a sensitive and specific method suitable for routine work. The improved resolution of the capillary column (compared to packed columns) provides well resolved peaks which result in cleaner mass spectra and thus more certain identification of the various volatile compounds. However, capillary columns are not the answer for every analytical problem.
- Basic priority pollutants were not found in the industrial effluents using SE-30 glass capillary columns. Benzidine and 3,3'-dichlorobenzidine could only be detected reliably at levels of greater than 50 µg/l with our method. Consequently, if lower detection limits are necessary for benzidine analysis, more suitable methods should be used. One such method is the electrochemical detection of benzidines following HPLC separation.
- Mass spectral and relative retention time data bases containing most, if not all, of the organic compounds produced by industry should be developed. Present data bases contain mass spectra of less than 20% of the presently manufactured industrial compounds. Consequently, identification of "unknown" pollutants was difficult due to the incomplete data bases of the mass spectral matching systems. Manual

interpretation procedures are not feasible for a screening project of this scale.

- The majority of pollutants present at levels greater than 10 µg/l were tentatively identified. However, there is considerable uncertainty associated with some of the interpretations. In general the most common and most frequently studied compounds (i.e., hydrocarbons, halocarbons, fatty acids, and phenols) are identified with a high degree of certainty. Pollutants which have not been previously identified are of particular interest in this type of study but they are less likely to be included in data bases and less likely to be correctly identified.
- The Biemann computer mass spectral matching system does provide a useful "first guess" in the identification of an unknown compound, but it is unreliable in determining the degree of certainty of a particular compound identification. Thus, the computer generated GC/MS data alone are not sufficient evidence for the positive identification of "unknown" compounds. Retention time data and manual interpretation must be used.
- Many samples contained only a few components as determined by preliminary GC analysis, whereas others contained many compounds in high concentrations. Consequently, the GC screening procedure used (i.e., priority rating system) saved time and money by determining which samples contained a sufficient number of components above a specified concentration level (10 µg/l) to warrant subsequent GC/MS/COMP analysis. However, the relatively few contaminants present in those samples not analyzed by GC/MS may have been potentially toxic components that should be of concern.

ANALYTICAL RESULTS

- Caution should be used when interpreting the analytical data, especially the frequency of occurrence tables, because this was only a limited study.
- Generally, industrial effluents contain few priority pollutants. In the semivolatile fractions only 17 priority pollutants were identified and these occurred collectively 78 times--only 10% of the 816 occurrences of semivolatile compounds. This percentage of occurrence of priority pollutants is the upper limit since the unidentified compounds would not be priority pollutants.
- Priority pollutants are most prevalent in the purgeable fractions of industrial effluents. This was expected since most of these compounds are common industrial solvents. Twenty-two priority

pollutants were identified and occurred collectively 359 times-- 51% of the 710 occurrences of purgeable compounds.

- Most of the components found in the effluents were specific for a particular industrial site and did not appear in re-occurring patterns. Specifically, 176 out of 261 neutral compounds, 56 out of 104 acidic compounds, 39 out of 49 basic compounds, and 85 out of 159 volatile compounds occurred only once. These data suggest that many possible environmentally important compounds (mutagenic, toxic, carcinogenic) would be overlooked if frequency of occurrence is the major criterion for determining environmentally significant compounds.
- Few polycyclic aromatic hydrocarbons (PAH's) were identified in industrial effluents. This fact supports the combustion airborne hypothesis that PAH's enter the surface waters primarily as a result of the combustion of fossil fuels.
- Many different types of heterocyclic compounds appeared in the basic fraction. Such compounds are very likely toxic or mutagenic and may prove to be environmentally significant.

FUTURE STUDIES

- We recommend that future studies concentrate on basic compounds using suitable methods of identification and that appropriate tests for compound activity (toxicity, mutagenicity, carcinogenicity) be conducted.
- We recommend that future studies concerning the environmental impact of various compounds first identify which compounds are biologically active (toxicity, mutagenicity, carcinogenicity) and then apply suitable methods for their detection in the environment. This could be accomplished by fractionating extracts using liquid chromatography and screening the fractions by bioassay techniques (e.g., Ames mutagenicity assay, mammalian cell toxicity assay). Active fractions would be subfractionated and studied in detail to identify the biologically active components.
- The current study was concerned only with volatile and semi-volatile components. The many nonvolatile organic components that were undoubtedly present and which may be biologically active were ignored. We recommend that future studies include efforts to identify biologically active nonvolatile components. This could be accomplished most efficiently by combining liquid chromatographic fractionation and bioassay techniques with HPLC-MS and HPLC/IR studies.

SAMPLING

SITE SELECTION

The objective of sampling site selection was to develop a sampling design system which allowed the collection of representative, usable and statistically reliable data concerning the possible source of organic pollutants entering receiving waters. A preliminary list of 478 organic chemical manufacturing facilities was compiled and classified according to type of chemical industry. Sampling sites were chosen from this list using the following criteria:

- (1) Type of industry
- (2) Potential toxicity of anticipated pollutants
- (3) Production capacity of company
- (4) Willingness of company to permit sampling

In retrospect, the main factor for site selection was the willingness of the company to permit sampling. The other major criterion was the type of industry to be considered. These industries included all types of organic chemical manufacturers and even steel manufacturers because of their coal tar production. Table 1 summarizes the various types of chemicals produced by these companies.

Letters were sent to 250 corporations requesting permission to sample at some 450 sites. Each company was informed that data obtained from their water samples would not be identified with their respective company. In this way each company's identity will remain confidential. Approximately 10% of the corporations contacted refused to participate. Many corporations (94 out of 250) had sampling sites (100) which discharged into municipal treatment plants. These sites were not applicable for this project since only those effluents which were discharged directly into surface waters were of interest. Eighteen corporations requested that intake water be analyzed as well as effluent water. In this way, chemicals identified as being introduced via the intake water would not be erroneously attributed to the manufacturing operations.

SAMPLE COLLECTION AND PRESERVATION

Samples were collected from sites in Ohio, West Virginia, Pennsylvania, New Jersey, New York, Louisiana, Kentucky, Delaware, and Texas. In total, samples of 63 outfalls and 22 intakes (plant water supply) were collected.

TABLE 1. CHEMICALS PRODUCED BY COMPANIES SAMPLED

rubber processing chemicals	surfactants
plastics and resins	elastomers
dyes, color agents and pigments	catalysts and catalyst supports
aromatic hydrocarbons	polymers
surface-active agents	organic intermediates
tar, tar prods, petroleum prods.	synthetic fibers
carbon black	paints and varnishes
lecithin and derivatives	enzymes
aliphatic solvents	pulp and paper chemicals
medicinals or pharmaceuticals	silanes, silicones
industrial organic chemicals	leather finishes
organic acids and salts	chelating agents
fatty acids & derivatives	amines
organic surface coatings	printing inks
flavor and fragrance chemicals	peroxides
pesticides	chlorine compounds
epoxys	edible fats, oils, etc.
miscellaneous organic chemicals	synthetic rubbers

Samples were collected in such a way as to provide as representative a sample as possible from each sampling site. This required close coordination with facilities personnel to ensure that sampling was performed during a representative stage of the production cycle. In many cases effluents from the various operations of a particular plant were pooled and may have been subjected to purification treatment prior to discharge. These pooled samples averaged many of the periodic fluctuations in the composition of the effluents and permitted a grab sample to be taken which was reasonably representative of several hours of operation. For this reason and because grab sampling is by far the least costly method, grab samples were collected at all the sites. Other advantages of grab sampling are that contamination is minimized and the sample can be immediately capped and cooled to prevent loss of volatile compounds.

Grab samples for analysis of semivolatile compounds were collected in pre-washed one-half gallon glass bottles containing 5 grams of potassium bisulfate (KHSO_4) and 75 grams of sodium chloride. Two bottles of sample were collected at each intake (or process water source) and process water outfall. Each bottle was filled approximately half full with sample water. Next, 150 ml of high purity distilled-in-glass methylene chloride was added followed by the remaining half portion of sample water. The methylene chloride prevents microbiological degradation and retards hydrolytic degradation of many organic components by removing them from the aqueous phase. A field blank was collected at each site in the same manner as a sample using distilled water (taken to each site from the laboratory) instead of waste or inlet water. All bottles were appropriately labelled and stored on ice.

Grab samples to be analyzed for volatile compounds were collected in 40 ml glass vials. Four samples were collected at both the inlet and outfall by filling each vial until it overflowed. This sampling method ensured that no air remained in the samples. The completely filled vials were sealed with screw-caps containing Teflon-lined silicon rubber septa and stored cap-side down on ice. A field blank consisting of distilled water was prepared at each site using the preceding overflow method. All water samples were stored at 4°C until they were extracted and/or analyzed by GC/MS.

SAMPLE ANALYSES

All sample analyses involved a GC/MS/COMP system that used high-resolution glass capillary GC columns. Volatile compounds were purged from water by helium, trapped on Tenax and subsequently desorbed. Semivolatile compounds were extracted from water with methylene chloride using an extraction scheme that gave the neutrals, acids, and bases as three separate fractions. These three fractions were analyzed by GC as well as by GC/MS/COMP.

INSTRUMENTATION

A Tekmar Liquid Sample Concentrator, Model LSC-1, was used for purging the volatile compounds. The device was equipped with a 25-ml sample container and the adsorbent tube was packed with 6 inches of 60/80 mesh Tenax GC. A 25-ml gas tight syringe with a 3-way valve and 12-inch needle was used to transfer the water samples to the LSC-1.

The GC/MS system for both the volatile and semivolatile analyses consisted of a Finnigan Model 9500 gas chromatograph coupled with a Finnigan Model 3200 quadrupole mass spectrometer. The mass spectrometer was interfaced to a Systems Industries Model 150 data system.

The GC column for volatile analyses was a 50 m x 0.25 mm i.d. glass capillary column (Perkin-Elmer) coated with SF-96 (a low molecular weight methyl silicone fluid). Figure 1 illustrates the instrumentation used in our purge and trap method.

The GC analyses of semivolatile compounds were performed using a Varian Model 1840 or Hewlett-Packard Model 5730 gas chromatograph equipped with a Hewlett-Packard automatic sampler. Each GC was fitted with a 30 m x 0.22 mm i.d. SE-30 glass capillary column (J. & W. Scientific). The calculation of retention index and concentration relative to the internal standard (pentadecylbenzene) was performed by a Spectra-Physics Model 4000 chromatography data system.

VOLATILE ANALYSIS PROCEDURES

During the course of this project it was mutually decided with the sponsor that all 85 samples would be analyzed for volatile compounds by using capillary column GC/MS instead of the usual packed column GC/MS system. The employment of capillary column GC/MS for routine volatile analyses proved to be a significant technical improvement in this project by providing well resolved GC peaks which result in clean mass spectra of volatile compounds.

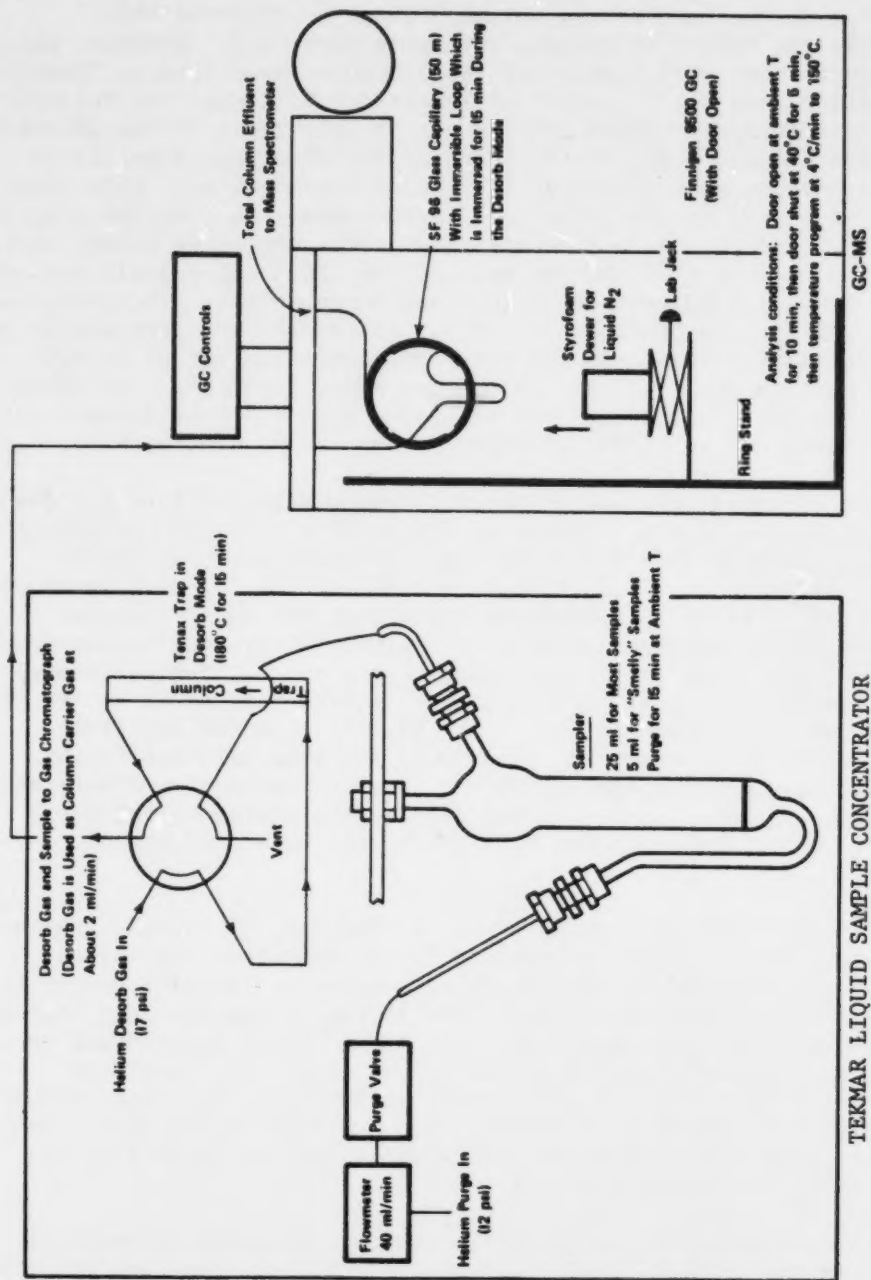


FIGURE 1. INSTRUMENTATION FOR PURGE AND TRAP ANALYSIS

Experimental Method

Since the glass capillary column was attached directly to the mass spectrometer, cryogenic trapping was used to concentrate the entire volatile sample as a plug on the head of the column. Thus no compounds were pumped away with the helium by passing through a separator. However, this method did require some modification of the procedure described in "Sampling and Analysis Procedures for Screening of Industrial Effluents for Priority Pollutants".(1) One modification was the use of only Tenax in the adsorbent tube. If silica gel was added at the front of the adsorbent tube, large amounts of water vapor were eluted during the desorption step. This water sometimes formed a plug in the glass capillary column. In a second modification, the LSC-1 Desorb Mode outlet was used as the capillary column carrier gas. The helium entered a "T" at the back of the LSC-1 and a small pressure regulator was installed between the Desorb and Purge inlets. The pressure was set at 15 psi for the Desorb inlet (i.e., 15 psi was the pressure at the head of the capillary column) and the purge regulator was set at 12 psi. The flow rate through the capillary column was about 3 ml/min. The first coil of the glass capillary column was fashioned into a U-tube about 4 cm deep which was immersed in liquid nitrogen during the desorption step.

To analyze a sample, 25.0 ml of water sample was poured into the gas-tight syringe followed by the addition of 200 μ l of a solution containing 200 ng of the internal standard (the internal standard was prepared by diluting 74 μ l (100 mg) of 1,2,3-trichloropropane to 10.0 ml with methanol and then diluting 10 μ l of this solution containing 100 μ g of internal standard to 100 ml with sparged water); this gives an internal standard concentration of 8 μ g/l. The sample was added to the purging device through a septum and sparged for 15 min with helium at a flow rate of 40 ml per min. The Tenax trap was then desorbed for 15 min at 180° with the capillary U-tube immersed in liquid nitrogen. The LSC-1 was then switched to the Purge mode, the liquid nitrogen was removed from the capillary column, and data acquisition started. A plug of air reached the source in the mass spectrometer in about three minutes followed by the separated organic components.

The GC/MS conditions were as follows: 1) the initial column temperature was 25°C and held at this temperature for 10 min after the solvent front (air) passed through the column; 2) the column was quickly heated to 40°C and held at this temperature for 5 min; 3) the column was then temperature programmed at 4°C/min to 130°C and held at the final temperature until all the volatile components eluted (usually 10-15 min); 4) the MS was scanned from m/e 40-350 with the sensitivity at 10^{-7} and the electron multiplier voltage at about -2.00 KV. Between each run the purging device was rinsed several times with sparged distilled water and the Tenax trap was baked out at 210°C for 15 minutes.

2-Bromo-1-chloropropane was initially used as the internal standard. However, experiments revealed that the 2-bromo-1-chloropropane was not completely resolved from toluene and also exhibited two isomer peaks on the

SF-96 capillary column. Consequently, 1,2,3-trichloropropane was used as the internal standard. The internal standard (200 ng) was added to each sample including the blanks and reference solutions. Retention times relative to 1,2,3-trichloropropane were calculated for each compound found in the samples. Figure 2 shows a typical RGC of the volatile components in an industrial wastewater samples.

Quantitation

The quantitation of each volatile compound using extracted ion currents of major ions of each compound would be time consuming (computer time) and costly. Therefore, it was mutually agreed with the sponsor that a semi-quantitative estimation of the amount of each volatile component found would be adequate for this program. Relative peak heights of reference compounds (i.e., response factors) in the normalized total ion chromatogram (T.I.C.) were used to estimate the concentrations of each compound in the samples. The relative responses of acetone, diethyl ether, benzene, chlorobenzene, and o-xylene (compounds which appear in many of the industrial samples) were determined to be in a 20-fold range and depended upon the stripping efficiency of the procedure (related to compound solubility and volatility) and the ionization and chromatographic characteristics (polarity, molecular weight, etc.) of the compounds. For compounds identified in the samples, estimated relative response factors were used to estimate the approximate quantity of each compound. Initially, relative responses for a few samples could not be obtained because the sample components were so concentrated that the internal standard peak was not observed in the normalized TIC plot. Consequently, three additional internal standards (bromochloromethane, 2-bromo-1-chloropropane and 1,4-dichlorobutane) were added to all samples. This modification permitted reliable semi-quantification of the volatile compounds in the industrial water samples. Table 2 lists the relative responses of internal and external standards used in our semi-quantification of volatile compounds.

SEMIVOLATILE ANALYSIS PROCEDURES

Each of the 85 water samples was extracted to give three fractions containing the neutral, acidic, and basic semivolatile compounds, respectively. These fractions were gas chromatographed (methylated acid fraction) to obtain semiquantitative data and to prioritize the respective fractions for subsequent GC/MS/COMP analysis. Only the top priority fractions (total of 89) were analyzed by GC/MS/COMP.

Experimental Method

Semivolatile organic compounds were extracted from each water sample using the procedure illustrated in Figure 3.

Each 1500 ml sample, previously treated with 5 g of KHSO_4 and 75 g of NaCl , was spiked with three internal standards--hexaethylbenzene, 2,4-dimethylaniline and palmitic acid. The pH was adjusted to $\text{pH} \approx 1$ using H_2SO_4 and the sample extracted three times with nanograde distilled in glass

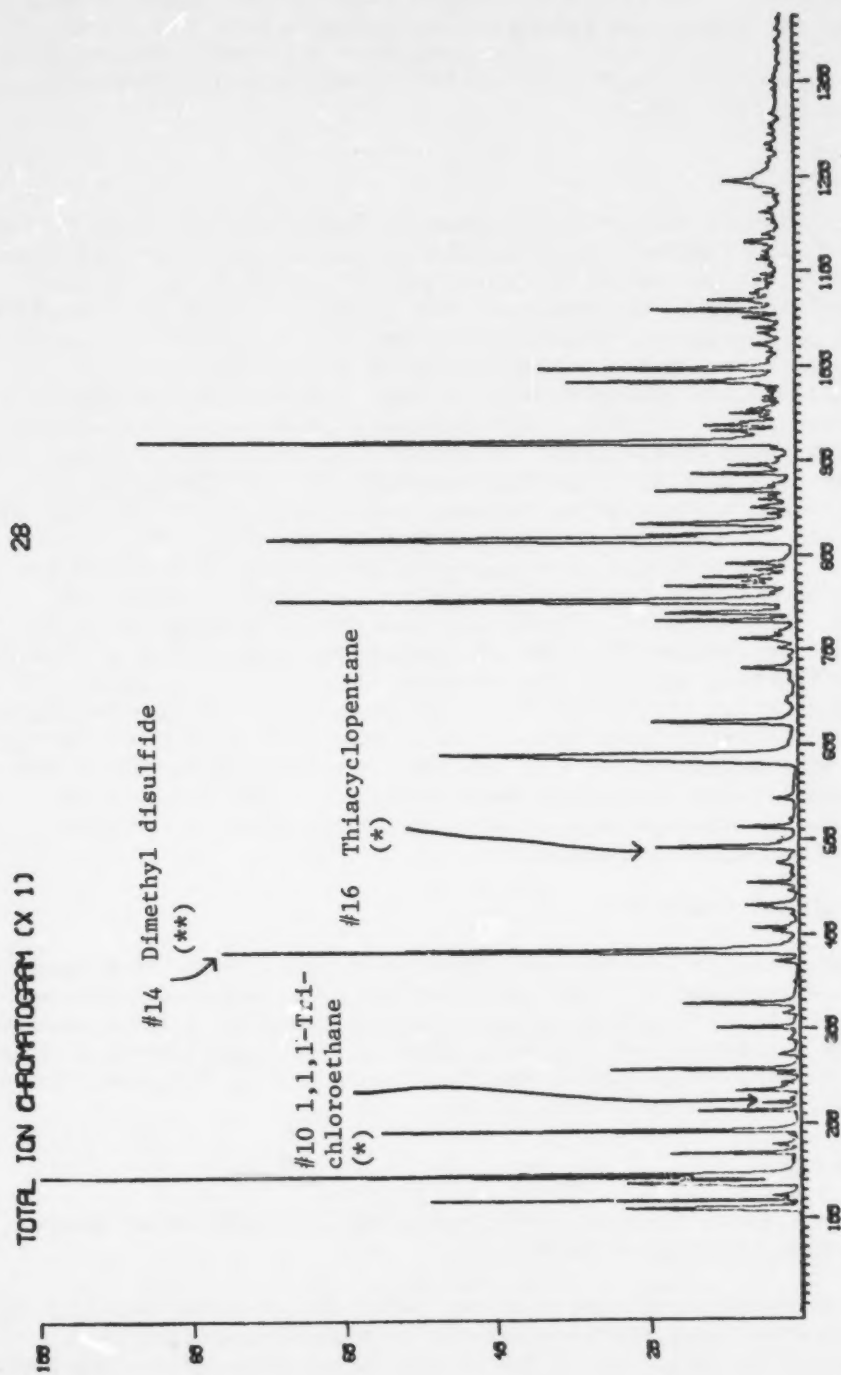


Figure 2. Total ion chromatogram of volatile fraction of industrial effluent.

TABLE 2. INTERNAL STANDARDS AND EXTERNAL STANDARDS

Compound	Amount in 25-ml water sample, ng	Concentration, $\mu\text{g/l}$	Relative Response ^a
Acetone	473	19.0	0.8
Diethyl ether	142	5.7	7.3
Benzene	178	7.0	11.5
Chlorobenzene	221	8.8	3.2
o-Xylene	176	7.0	3.8
Bromochloromethane	200	8.0	5.0
2-Bromo-1-chloropropane	200	8.0	3.9
1,4-Dichlorobutane	200	8.0	1.1
1,2,3-Trichloropropane	200	8.0	1.0

(a) Response/concentration relative to that of the internal standard, 1,2,3-Trichloropropane

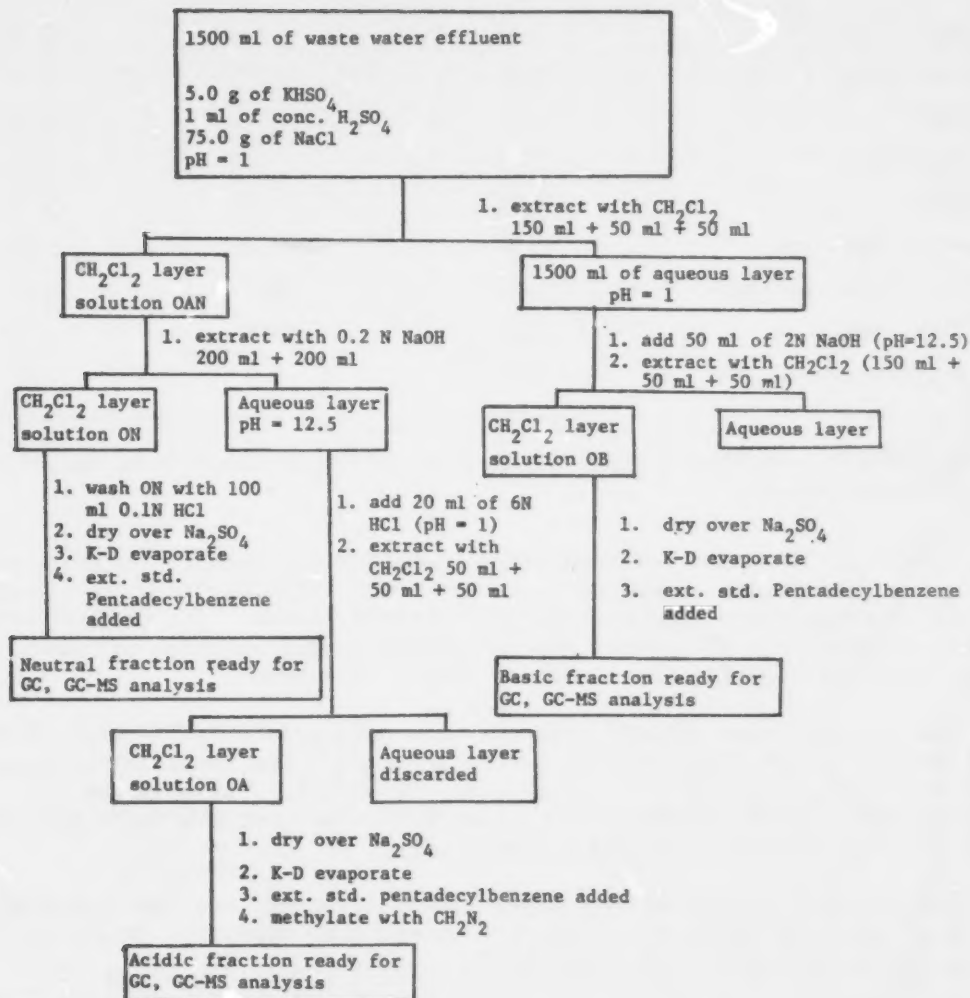
methylene chloride. The combined methylene chloride extracts (neutral and acidic fractions) were extracted twice with 0.2N NaOH resulting in organic (neutral fraction) and aqueous (acidic fraction) layers. The organic layer was washed with 0.1N HCl, dried over anhydrous sodium sulfate, filtered, and concentrated to 400 μl using a Kuderna-Danish evaporator.

The aqueous layer (acidic fraction) was made acidic ($\text{pH}\approx 1$) with 6N HCl and extracted three times with methylene chloride. The resulting organic layer was dried, filtered and concentrated to 400 μl . The solution was split in half. Half was methylated using a diazomethane generator and the other half was stored for possible reanalysis.

The original acidic aqueous layer (basic fraction) was made alkaline, ($\text{pH}\approx 12.5$) using 2N NaOH, extracted three times with methylene chloride, dried, filtered, and concentrated to 400 μl .

An internal standard, 20 μg of pentadecylbenzene was added to each of the respective fractions together with 400 μl of benzene. Each fraction was concentrated to 400 μl , split in half and stored at 4°C until GC or GC/MS analysis. By replacing methylene chloride with the higher boiling solvent benzene, samples had longer storage life. More importantly, the "solvent effect" produced by benzene improved column resolution and peak shape in subsequent splitless injections of GC/MS analyses.

FIGURE 3. EXTRACTION PROCEDURE



All 255 fractions were analyzed by GC using the conditions listed in Table 3.

TABLE 3. GAS CHROMATOGRAPHIC CONDITIONS*

Injection procedure	2 μ l 10:1 split
Initial temperature	60°C
Initial time	5.0 min.
Programming rate	4°C/min.
Final temperature	260°C
Final time	35 min.
Injector temperature	250°C
Detector temperature	300°C

*30 m x 0.22 mm i.d. SE-30 glass capillary column.

Figures 4, 5 and 6 illustrate typical gas chromatograms of the respective neutral, acidic, and basic fractions from industrial waste-water effluents. The GC/MS conditions for semivolatile compound analysis were similar except that a 2 μ l splitless injection was used.

Quantitation

The emphasis of this program was on the identification and not quantification of organic compounds. Consequently, semiquantitative methods based solely on gas chromatography were sufficient. The Spectra-Physics 4000 data system calculated concentrations using pentadecylbenzene as an internal standard. The sample component concentrations were calculated using "estimated response factors" which were obtained by correlating the following:

- (1) The relative response of a similar compound found in the BCL Standard Mixtures (Table 4);
- (2) The recovery of the respective fractions (determined by comparison of internal with external standard);
- (3) The shape of the respective GC peak and baseline (which indicated how accurately each peak area was integrated).

The reliability of our quantitative data depended ultimately upon the computer integration of the respective GC peak areas. Because of actual problems associated with this procedure (co-eluting compounds, poor GC peak shape and/or irregular baseline), the following ranges were established for reporting compound concentrations:

- (1) * = less than 10 μ g/l
- (2) ** = 10-100 μ g/l
- (3) *** = greater than 100 μ g/l.

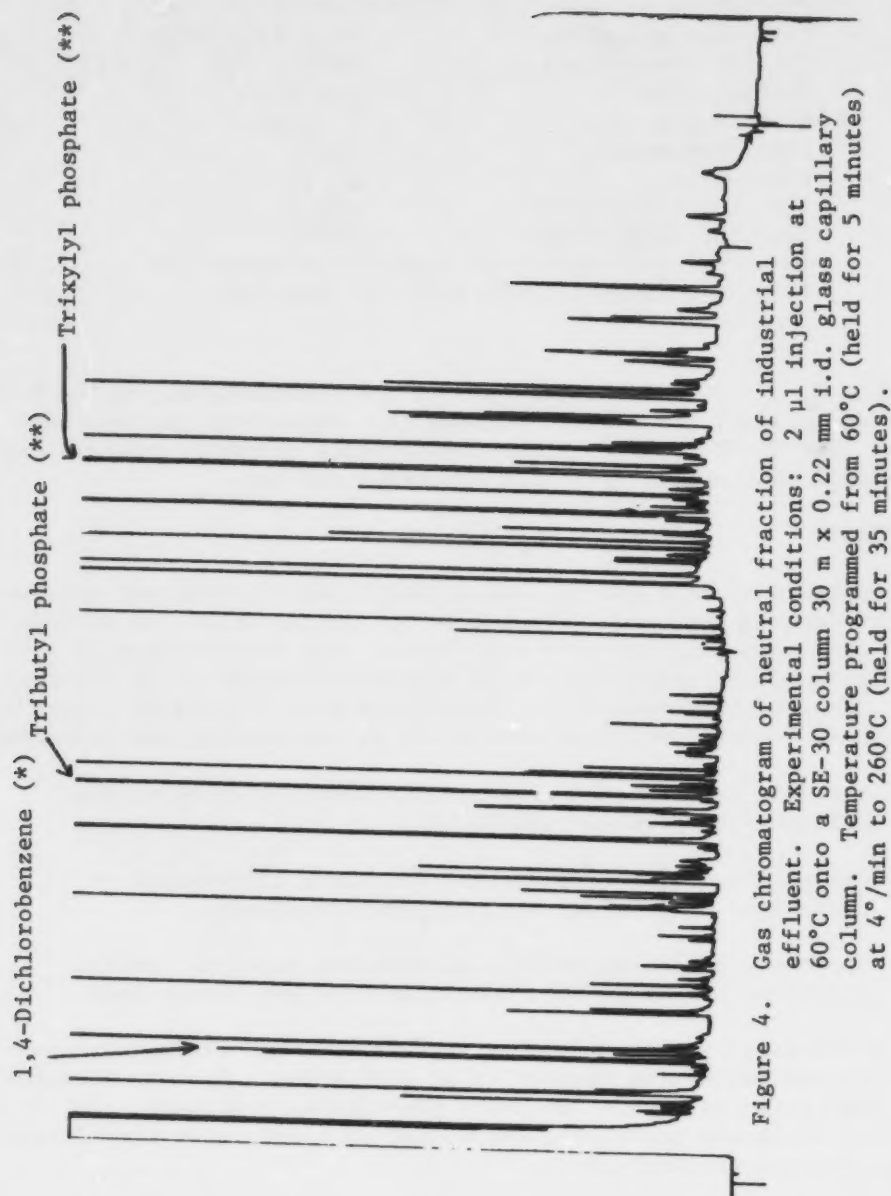


Figure 4. Gas chromatogram of neutral fraction of industrial effluent. Experimental conditions: 2 μ l injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes).

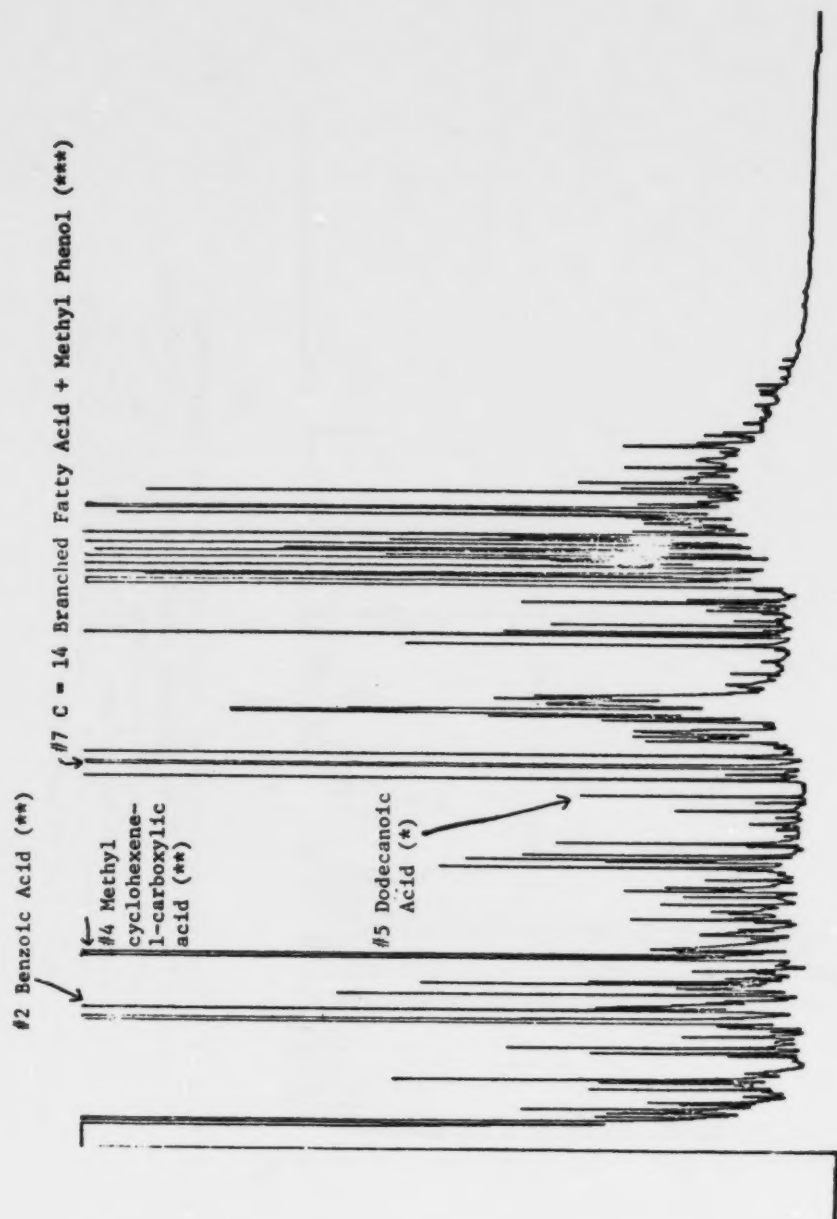


Figure 5. Gas chromatogram of acidic fraction of industrial effluent. Experimental conditions: 2 μ l injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes).

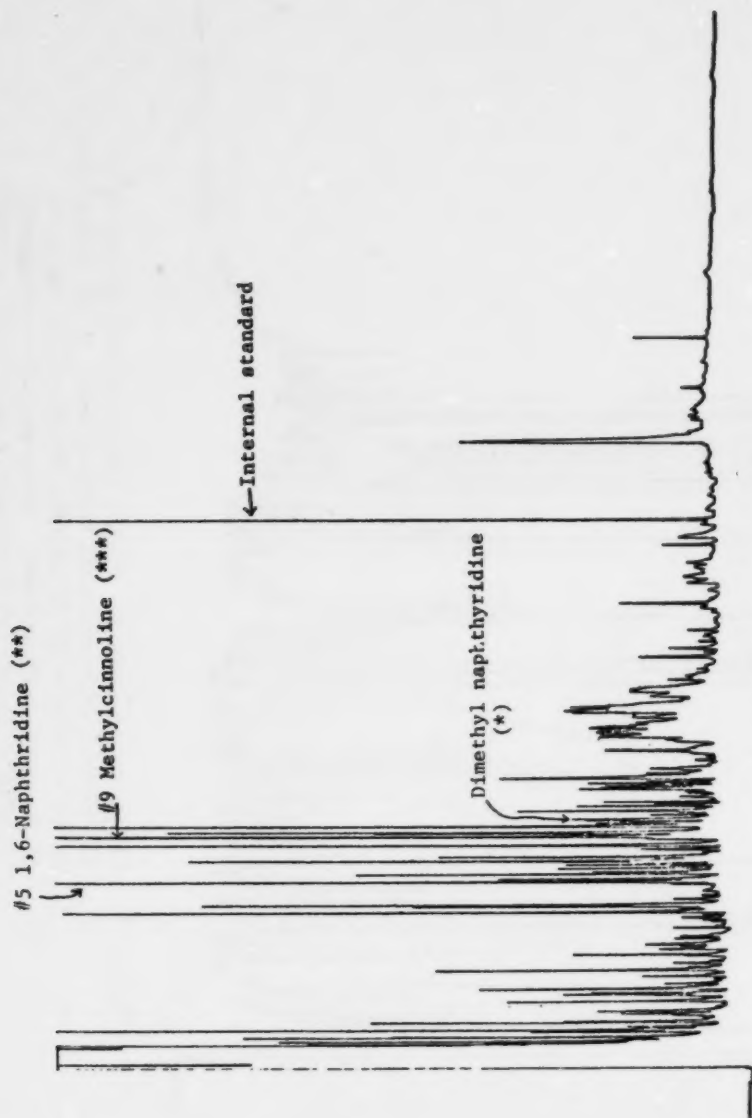


Figure 6. Gas chromatogram of basic fraction of industrial effluent. Experimental conditions: 2 μ l injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes).

Table 4. Recovery of Compounds in BCL Standard Mixture

Compound	No. of Runs	Recovery, %	Relative Standard Deviation, %
1. Chlorobenzene	4	94.3 $\pm$ 8.7	9.2
2. Nonane	4	87.9 $\pm$ 9.5	10.1
3. 1,2,4-Trimethylbenzene	4	98.9 $\pm$ 8.1	8.1
4. Naphthalene	4	88.4 $\pm$ 7.2	8.1
5. Decylaldehyde	4	88.7 $\pm$ 11.0	12.4
6. Dibenzofuran	4	93.0 $\pm$ 4.6	4.9
7. Tri-n-butyl Phosphate	4	85.8 $\pm$ 5.2	6.0
8. Pentadecanol	4	155.8 $\pm$ 60.8	39.0
9. Dibutyl Phthalate	4	85.1 $\pm$ 9.4	11.0
10. Carbazole	4	131.0 $\pm$ 12.9	9.8
11. Pyrene	4	88.6 $\pm$ 12.2	13.7
12. Methyl Stearate	4	82.8 $\pm$ 8.4	10.1
13. Heptadecylcyclohexane	4	79.0 $\pm$ 9.0	11.3
<u>Acidic Fraction</u>			
1. 2,6-Dimethylphenol	5	97.5 $\pm$ 8.1	8.3
2. p-Nitrophenol	4	26.6 $\pm$ 3.4	12.7
3. m-Nitrobenzoic Acid	4	45.2 $\pm$ 20.4	45.0
4. 2,3,4,5-Tetrachlorophenol	5	97.0 $\pm$ 7.2	7.4
5. Palmitic Acid	5	118.8 $\pm$ 15.8	13.4
<u>Basic Fraction</u>			
1. N-Ethylmorpholine	5	98.9 $\pm$ 8.4	8.4
2. Dibutylamine	2	70.5 $\pm$ 9.6	13.6
3. 2,4-Dimethylaniline	5	94.9 $\pm$ 14.4	15.1
4. Quinoline	5	109.5 $\pm$ 6.8	6.2
5. m-Nitroaniline	5	72.4 $\pm$ 11.8	16.3

QUALITY ASSURANCE STUDIES

An essential and enlightening aspect of this project was the continued use of various quality assurance measures. Because of the variety of chemical and physical properties of compounds expected to be found and the $\mu\text{g/l}$ detection limit, stringent standards were necessary to validate our procedures for the extraction, detection, and identification of compounds from industrial wastewater effluents. These quality assurance standards included instrumental calibration, recovery studies, and process and field blank studies.

Gas Chromatograph Calibration

A standard solution containing 2,6-dimethylphenol (DMP), 2,4-dimethylaniline (DMA), decylaldehyde, decanol, *n*-tridecane, and *n*-tetradecane was injected into the GC to determine the polarity, separation number (SN), and number of effective plates (N_{eff}) of the glass capillary column. This evaluation was made each time a column was connected in the GC and each time column degradation was suspected. In order for a GC column to have been acceptable for sample analysis the following conditions had to be met.

- (1) $N_{\text{eff}} \geq 50,000$
- (2) $\text{SN} \leq 25$
- (3) $\text{Area of DMP/Area of DMA} = 0.5 \text{ to } 2.0$
- (4) Width of half height for decanol $\leq 4 \times$ width at half height for tridecane.

In addition, a mixture containing C_9 to C_{32} *n*-paraffins was analyzed periodically to calibrate the retention time in terms of retention index (R.I.). This retention index calibration was made each time a column was connected in the GC and each time the retention index of the internal standard changed by 4 units relative to the previously calibrated value. A typical gas chromatogram obtained by the injection of this calibration standard mixture is shown in Figure 7.

GC-MS-COMP Calibration and Evaluation

The GC-MS-COMP system is checked daily by injecting a tune-up standard mixture and employing the following procedures and criteria.

Mass Spectrometer Tune Up

- (1) Adjust zero level of the mass spectrometer using a preamplifier setting 10^{-8} amp/volt, and the filament (800 μA) and electron multiplier ($\sim 2\text{kV}$, gain $\sim 5 \times 10^4$) on.

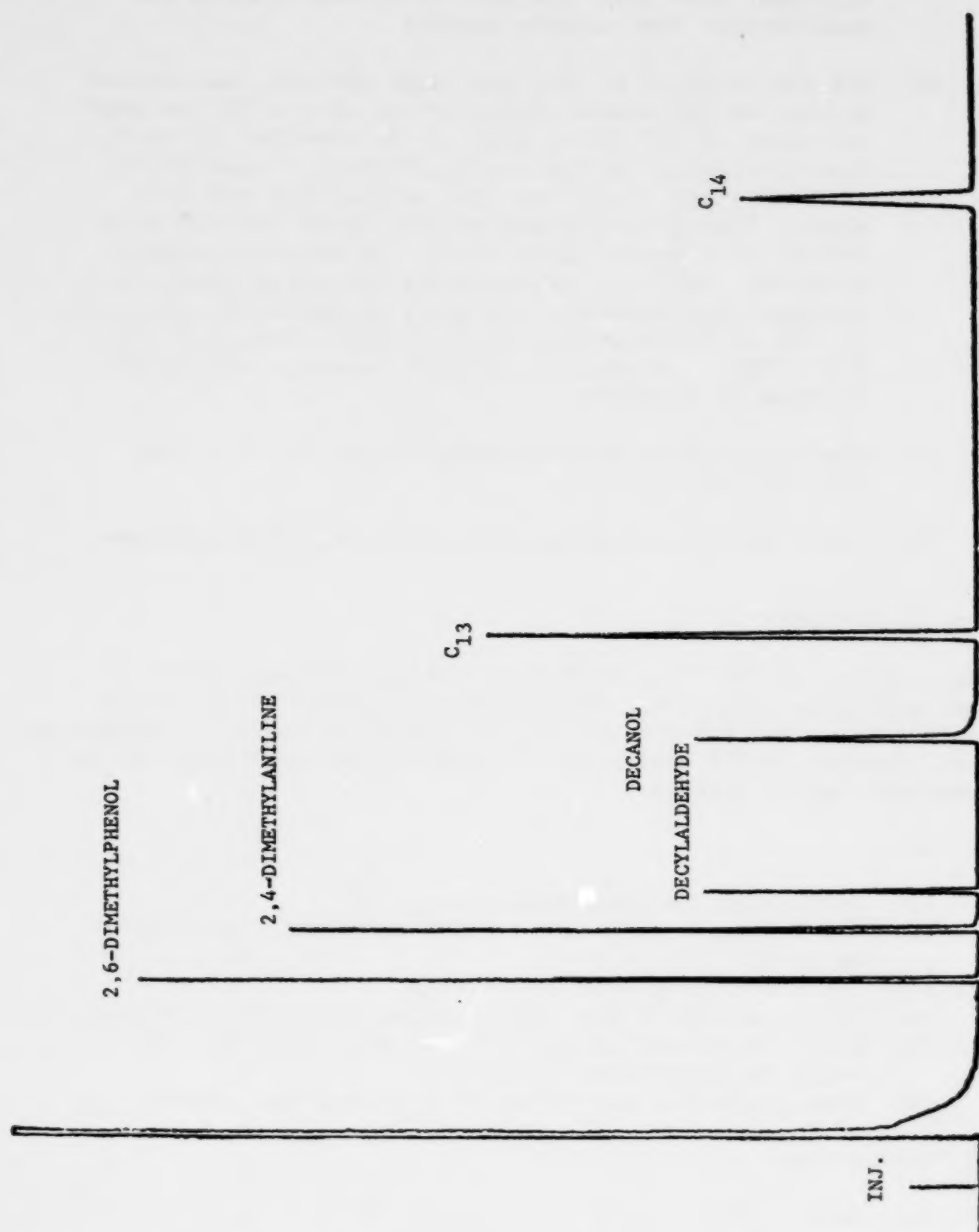


Figure 7. Glass capillary gas chromatogram of the calibration standard used for non-polar columns.

- (2) Admit FC-43 into the ion source and tune the MS as follows:
- (a) Using the potentiometers on the "Ion Source Controller", optimize the electronics to give highest intensity with best peak shape for m/e 219 as described by the manufacturer (see service manual).
 - (b) Set the controls to scan the range 400-600, and further adjust the ion source controller to give a 219 ion peak intensity of ~50-70% of that of the repeller to ~10 V, then decreasing the ion energy slightly. Again focus on m/e 219 and adjust the lens voltage for good peak shape. Tuning in this manner will favor the high mass end of the spectrum (i.e. >200). Decafluorotriphenylphosphine (DFTPP) is admitted via the solids probe into the mass spectrometer. Its spectrum should be comparable to that of Eichelberger, et al. [(Anal. Chem., 46 (7), 995 (1975))]. A spectrum of DFTPP taken in this manner is shown in Figure 8.
 - (c) Check peak shape and resolution at 18, 69, 219, 264, 414, and 502.
 - (d) Check calibration using CONT mode using 10 samples/amu.

GC-MS Tune Up Mixture

Inject 1.0 μ l of the "Tune Up Mixture" using a syringe with a 4" needle and splitless techniques. This mixture contains 30 ng each of 2,4-dimethylaniline and 2,6-dimethylphenol, and 10 ng each of 1-octadecene, octadecane, phytane, DFTPP, and methyl stearate. The conditions of the GC and computer are as follows:

- (1) GC
 - (a) Cool column to room temperature
 - (b) Set initial temperature to 20°C and final temperature to 200°C
 - (c) Set the program rate to 20°C/min
 - (d) Inject 1.0 μ l of the mixture using splitless techniques
 - (e) When the solvent elutes into the mass spectrometer, begin the temperature program
 - (f) Data collection can begin after solvent has passed
- (2) Data System
 - (a) Mode: IFSS
 - (b) Max repeat count: 5
 - (c) Integration time: 2
 - (d) Check lower threshold: 2
 - (e) Lower threshold: 3

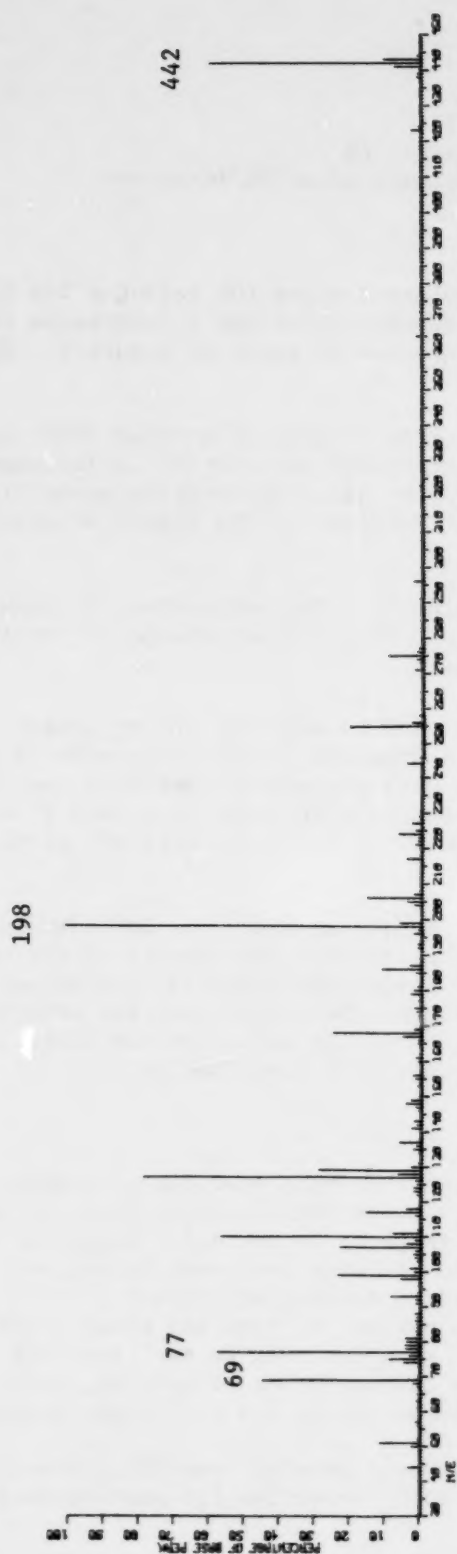


Figure 8. Electron impact mass spectrum of DFTPP

- (f) Upper threshold: 1
- (g) Clock: Y
- (h) Fast scan opt: Y
- (i) Delay between scans: CR
- (j) Start clock 10 seconds after GC injection

GC-MS-Comp Evaluation

The resulting data were evaluated using the Selected Ion Summation Program (SIS) and plotting the Reconstructed Gas Chromatogram (RGC). A typical SIS reconstructed chromatogram is shown in Figure 9. The following parameters were evaluated:

- (1) Capillary column pH - Peak heights of aniline (DMA) and phenol (DMP) were equal if the column was neutral; a decrease in aniline indicated an acidic column and a decrease in phenol indicated a basic column. Area of DMP/Area of DMA should be within the range of 0.5 to 2.0.
- (2) Capillary column resolution - The hydrocarbon GC peaks were used to evaluate resolution. The GC peaks should be resolved with no more than a 50% valley.
- (3) MS Tuning - DFTPP was used to evaluate the MS tuning under dynamic conditions. A spectrum on the front side of the DFTPP GC peak (before peak maximum if possible) was observed using CRTPLT. Eichelberger's criteria were used to evaluate this spectrum. A summary of these criteria are given in Table 5.
- (4) GC/MS transfer line - Methyl stearate was included in the mixture to evaluate the transfer line system of the GC/MS. When the transfer line was inadequately heated, the methyl stearate peak tailed. Obtaining a symmetrical peak for methyl stearate verified that large, involatile molecules can elute from the capillary column into the mass spectrometer.

Recovery Studies

For the semivolatile compound recovery studies, 13 neutral compounds, 5 basic compounds and 5 acid compounds (BCL Standard Mixture, see Table 4) were selected to ensure a wide range of GC retention times and different functional groups. Recovery studies were performed by analysis of process blanks spiked with the BCL Standard Mixture at a level of 13.3 $\mu\text{g/l}$. Two process blanks were analyzed in one set of runs and three process blanks were analyzed in another set of runs one week later. Recovery data are given in Table 4. Representative gas chromatograms of neutral, basic and acidic process blanks are shown in Figures 10, 11 and 12, respectively.

For most compounds, recovery was greater than 80%. Coeluting contaminants accounted for excessively high recoveries for pentadecanol and carbazole.

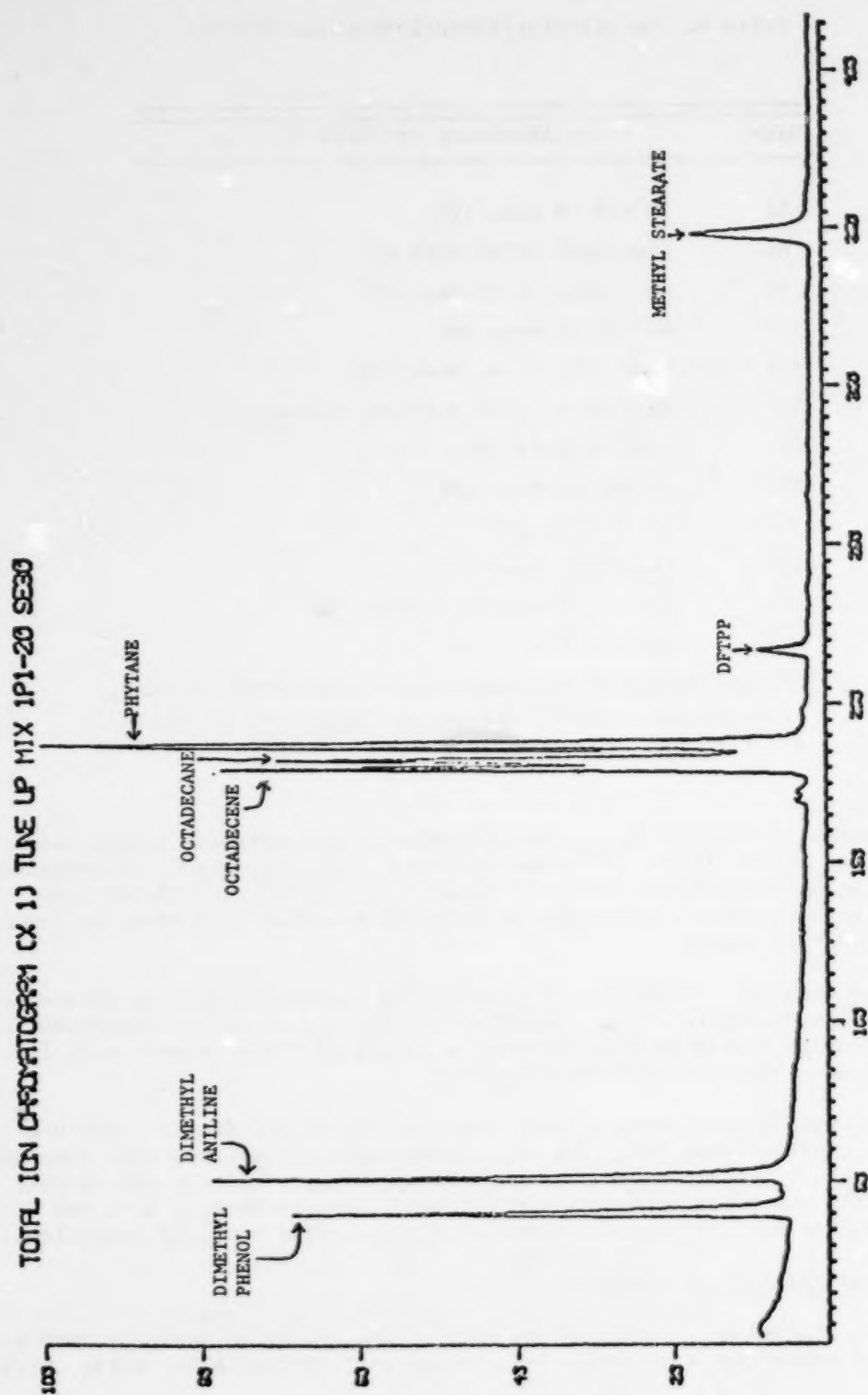


Figure 9. GC-MS-COMP tune up mixture chromatogram on a 30M SE30 capillary column

Table 5. Decafluorotriphenylphosphine (DFTPP)

Mass	Ion Abundance Criteria
51	30-60% of Mass 198
68	Less than 2% of Mass 69
70	Less than 2% of Mass 69
127	40-60% of Mass 198
197	Less than 1% of Mass 198
198	Base peak, 100% relative abundance
199	5-9% of Mass 198
275	10-30% of Mass 198
365	1% of Mass 198
441	Less than Mass 443
442	Greater than 40% of Mass 198
443	17-23% of Mass 442

Eichelberger, et al., Analytical Chemistry, 47 (7) 995 (1975).

Two compounds, p-nitrophenol and m-nitrobenzoic acid gave low recoveries, 27% and 45%, respectively. This was expected since these two acid compounds are very polar and fairly soluble in water. The reproducibility of the recoveries achievable is indicated by relative standard deviations of less than 15% in most cases.

As is true for all analytical programs, a continuing quality assurance program is necessary to ensure continued reliability of data. Consequently, weekly recovery checks carried out over a period of 4 months were made for this program. Table 6 lists these results.

The periodic recoveries of each compound in the BCL standard mixture generally averaged over 70%. The reproducibility of the respective recoveries was indicated by relative standard deviations of approximately 20% in most cases. Only the polar compounds p-nitrophenol, m-nitrobenzoic acid and m-nitroaniline had low recoveries and/or high relative standard deviations.

Process and Field Blank Studies

Blank studies were performed on each of the following reagents used in the sample collection and extraction procedures: CH_2Cl_2 , NaCl, KHSO_4 , Na_2SO_4 ,

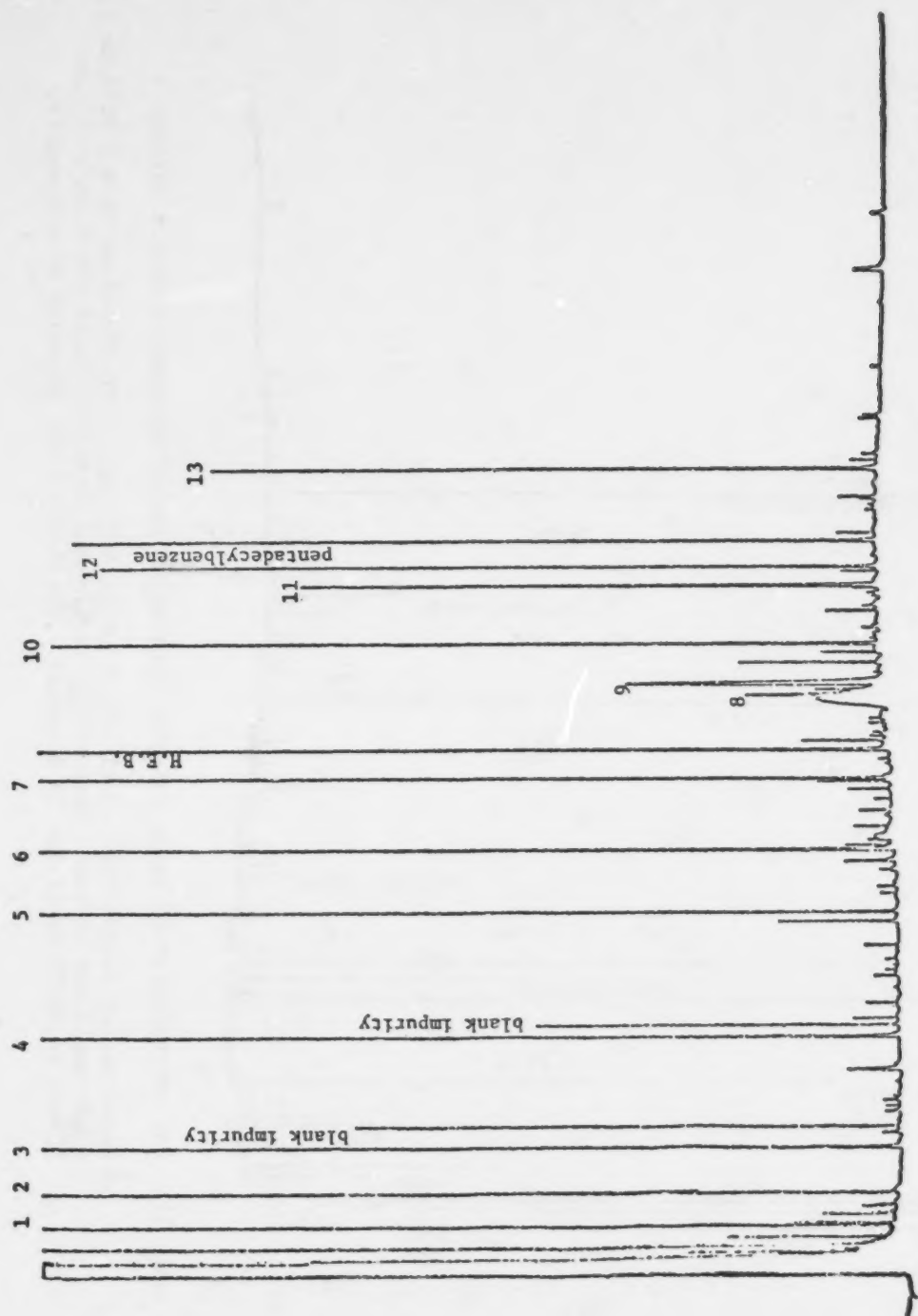


Figure 10. Gas chromatogram of neutral fraction from water spiked with BCL standard mixture

Experimental conditions: 2 μ l injection at 60°C onto a SE-30 column 3 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes). See Table 4 for identity of components.

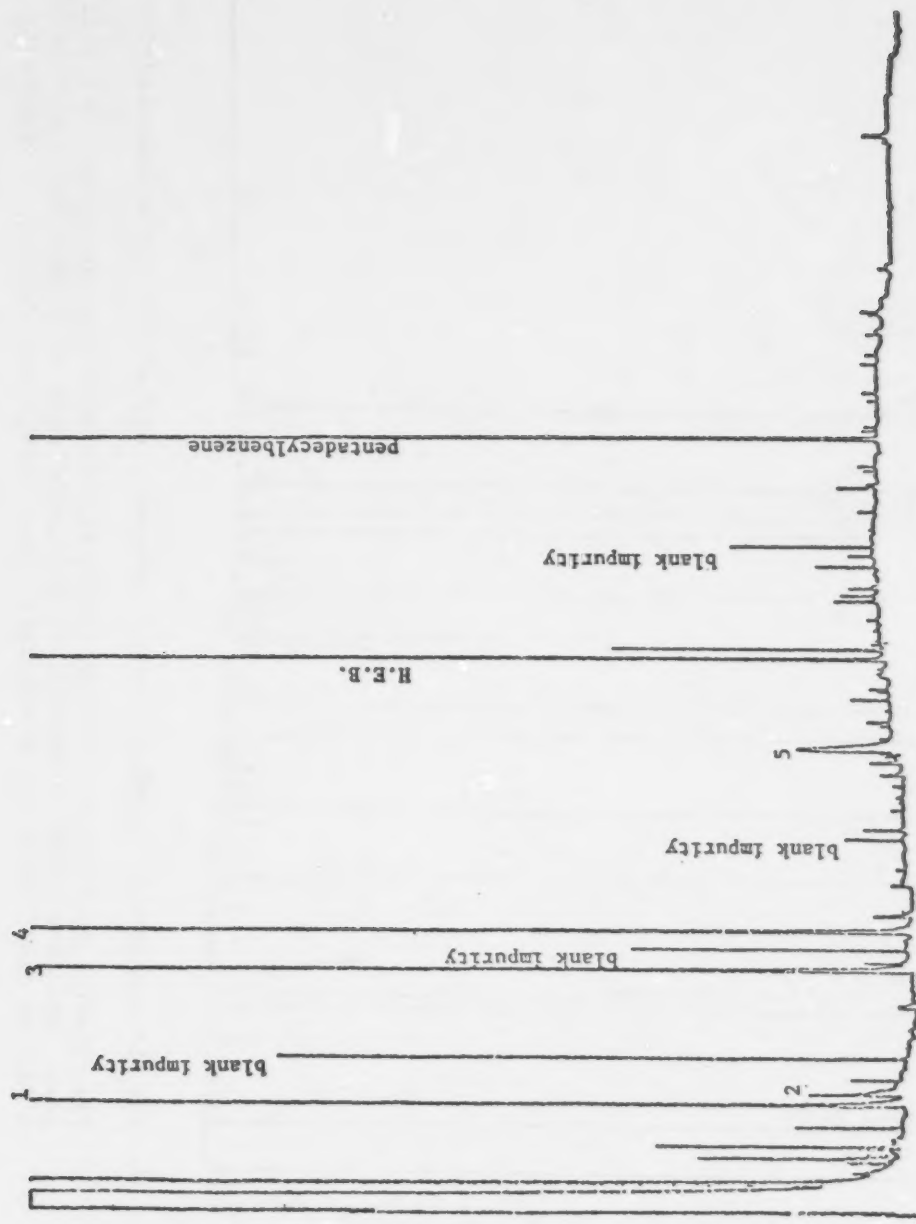


Figure 11. Gas chromatogram of basic fraction from water spiked with BCL standard mixture

Experimental conditions: 2 μ l injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes). See Table 4 for identity of components.

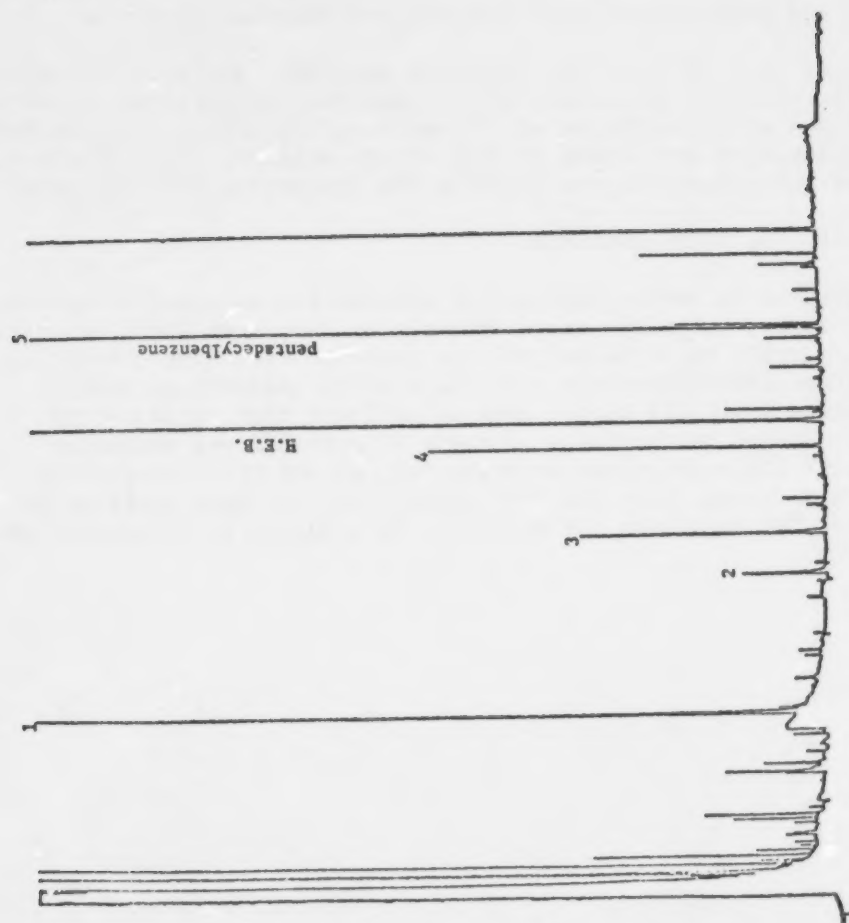


Figure 12. Gas chromatogram of acidic fraction from water spiked with BCL standard mixture

Experimental conditions: 2 μ l injection at 60°C onto a SE-30 column 30 m $\times$ 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes). See Table 4 for identity of components.

2N NaOH, 6N HCl, H₂O (millipore water). Methylene chloride was studied by 1000-fold concentration followed by GC analysis. All other reagents were extracted with CH₂Cl₂ which was then concentrated for GC analysis. Similar studies were carried out on the diazomethane generator, sample vials, filter paper, and Teflon liners (for vial caps). The GC results indicated that no contaminants from these sources were present at levels equivalent to <1 µg/l of water analyzed. Figures 13, 14, and 15 show typical examples of neutral, basic, and acidic process blanks, respectively.

Volatile sample blanks were generally run at the beginning of each day's analyses. The water used was previously sparged overnight with 50 ml/min of nitrogen at 50°C. The sparged water blanks generally yielded several small peaks (<1 µg/l) which probably are contaminants in the commercial distilled water. Figures 16, 17, and 18 show volatile sample process blanks and water spiked with internal and external standards.

Field blanks were obtained for each site sampled. Analysis of various field blanks for volatile and semivolatile compounds indicated no significant contamination occurred during any of our sampling procedures. Methylene chloride and chloroform were found in many of the volatile field blanks but at levels below the concentrations found in the respective effluent samples.

PRIORITY CRITERIA FOR GC/MS ANALYSES

In an effort to obtain as much useful information as possible within a limited budget it was mutually agreed with the sponsor that GC/MS analysis of semivolatiles would be performed only on selected fractions. Priority was given to those fractions which were shown by GC analysis to contain several components at levels higher than 10 µg/liter that could not be tentatively identified on the basis of their GC patterns and retention indices. Table 7 lists the three priority ratings and their respective criteria. In most cases, only the "++" rated fractions were analyzed by GC/MS. In total, 89 fractions (39 neutrals, 29 acidics and 21 basics) were analyzed by GC/MS.

Table 6. Periodic recovery of compounds in BCL standard mixture

Compound	Recovery, % From Spiked Process Blank Extracted on Given Date							
	12/27/77	1/3/78	1/11/78	1/23/78	1/31/78	2/6/78	2/9/78	2/13/78 2/20/78
<u>Neutral Fraction</u>								
1. Chlorobenzene	111	96.2	105	57.6	83.6	67.9	108.2	69.2 72.3
2. Nonane	106	95.5	96.0	50.5	74.4	55.6	80.9	26.3 60.9
3. 1,2,4-Trimethylbenzene	115	107	106	72.3	58.4	48.0	94.1	53.3 75.8
4. Naphthalene	108	99.5	108	87.9	74.9	73.1	104	81.8 80.2
5. Decylaldehyde	108	93.1	107	101	86.6	78.6	30.1	40.1 86.8
6. Dibenzofuran	116	105	114	103	71.5	76.7	98.1	105 84.9
7. Tri-n-butyl phosphate	108	85.4	118	110	104	118	98.7	125 82.5
8. Pentadecanol	114	125	106	118	109	115	69.5	104 80.0
9. Dibutyl phthalate	102	76.2	125	99.5	118	129	73.3	111 96.7
10. Carbazole	112	88.7	116	106	77.1	91.9	79.7	115 140
11. Pyrene	80.0	79.1	95.2	105	75.5	90.1	72.2	101 77.5
12. Methyl stearate	86.6	82.5	104	101	89.2	108	74.4	108 105
13. Heptadecylcyclohexane	76.0	71.3	96.4	98.8	78.3	84.1	78.3	81.2 84.4
14. Hexaethylbenzene	--	--	--	104	85.1	121	113	116 93.1
<u>Acidic Fraction</u>								
1. 2,6-Dimethylphenol	57.5	51.9	33.3	62.5	94.1	81.6	68.3	59.5 70.1
2. p-Nitrophenol	16.7	10.7	21.0	20.3	35.6	12.5	29.8	24.6 21.3
3. m-Nitrobenzoic acid	14.4	16.6	9.1	40.0	37.5	10.2	28.0	57.5 36.0
4. 2,3,4,5-Tetrachlorophenol	74.4	70.0	55.8	56.6	75.8	66.7	60.6	70.1 63.1
5. Palmitic acid	86.9	75.4	74.5	62.1	85.5	71.4	57.1	74.6 71.4
<u>Basic Fraction</u>								
1. N-ethylmorpholine	78.7	88.9	106	75.9	94.1	61.2	69.4	42.9 66.4
2. Dibutylamine	107	125	128	75.6	74.4	82.5	58.2	52.1 101
3. 2,4-Dimethylaniline	68.1	81.8	90.9	92.1	76.9	88.1	111	92.1 107
4. Quinoline	82.9	88.6	107	107	121	95.6	109	85.7 110
5. m-Nitroaniline	30.0	20.9	15.0	49.0	63.0	46.2	68.7	15.1 32.0

Table 6. (Continued)

Compound	Recovery, % From Soaked Process Blank Extracted on Given Date					Avg. $\pm$ Std. Dev. (%)	Relative Std. Dev. (%)	
	3/15/78	3/20/78	3/27/78	4/1/78	4/10/78			
<u>Neutral Fraction</u>								
1. Chlorobenzene	73.6	65.3	51.5	85.7	69.4	61.2	78.5 $\pm$ 18.3	23.3
2. Monane	82.6	73.8	55.0	61.7	60.1	86.9	71.1 $\pm$ 20.5	28.8
3. 1,2,4-Trimethylbenzene	94.1	82.2	68.8	92.1	84.1	109	84.0 $\pm$ 20.8	24.8
4. Naphthalene	93.1	80.0	73.8	68.3	59.2	63.3	83.8 $\pm$ 15.3	18.2
5. Decylaldehyde	80.5	82.4	69.1	53.7	60.2	57.9	75.7 $\pm$ 22.8	30.1
6. Dibenzofuran	88.8	83.6	93.2	95.3	54.2	50.8	89.3 $\pm$ 19.0	21.2
7. Tri-n-butyl phosphate	93.2	84.3	80.8	96.7	56.7	47.2	93.9 $\pm$ 21.2	22.5
8. Pentadecanol	102	79.3	80.3	48.5	42.2	37.5	86.6 $\pm$ 27.8	32.0
10. Carbazole	87.3	75.0	96.4	53.3	61.7	55.3	90.3 $\pm$ 23.8	26.4
11. Pyrene	76.6	68.2	73.4	55.6	61.1	57.1	77.8 $\pm$ 14.3	18.4
12. Methyl stearate	82.6	72.6	78.3	57.1	52.1	47.5	83.3 $\pm$ 19.4	23.2
13. Heptadecylcyclohexane	84.6	86.6	75.2	55.1	56.2	53.1	77.3 $\pm$ 13.3	17.2
14. Hexaethylbenzene	101	70.1	101	76.4	73.6	96.4	95.9 $\pm$ 16.3	17.0
<u>Acidic Fraction</u>								
1. 2,6-Dimethylphenol	75.1	75.0	96.7	55.1	83.3	33.3	67.8 $\pm$ 16.5	24.3
2. p-Nitrophenol	38.3	27.7	23.4	21.2	27.7	23.4	23.6 $\pm$ 7.3	20.9
3. m-Nitrobenzoic acid	46.0	40.0	44.0	19.0	14.0	16.1	28.5 $\pm$ 14.9	52.2
4. 2,3,4,5-Tetrachlorophenol	75.8	66.7	84.8	42.4	72.7	40.0	66.0 $\pm$ 11.9	18.0
5. Palmitic acid	74.6	74.3	71.5	44.3	65.7	41.0	68.7 $\pm$ 12.6	18.3
<u>Basic Fraction</u>								
1. n-Ethylmorpholine	88.0	92.5	88.0	120	108	80.0	84.0 $\pm$ 19.0	22.6
2. Dibutylamine	73.0	69.9	73.2	80.9	40.2	55.2	79.7 $\pm$ 24.8	30.1
3. 2,4-Dimethylaniline	85.0	68.3	66.7	123	96.4	64.3	87.4 $\pm$ 16.7	19.1
4. Quinoline	98.8	72.6	82.1	90.5	112	71.8	95.6 $\pm$ 14.5	15.2
5. m-Nitroaniline	31.4	20.1	28.6	40.0	40.2	14.3	34.2 $\pm$ 16.5	48.2

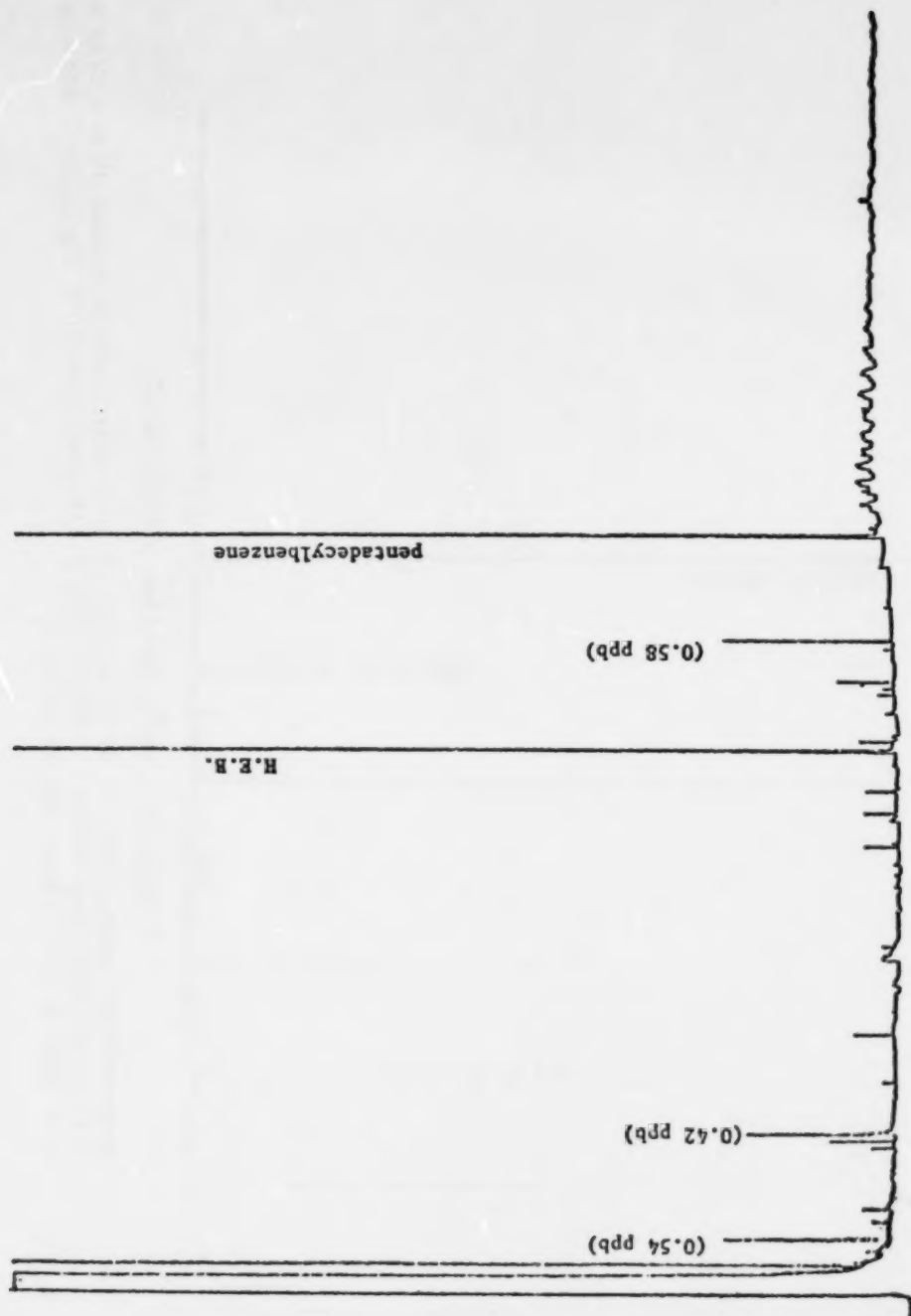


Figure 13. Neutral fraction process blank

Experimental conditions: 2 μ l injection at 60°C onto a SE-30 column 30m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes).

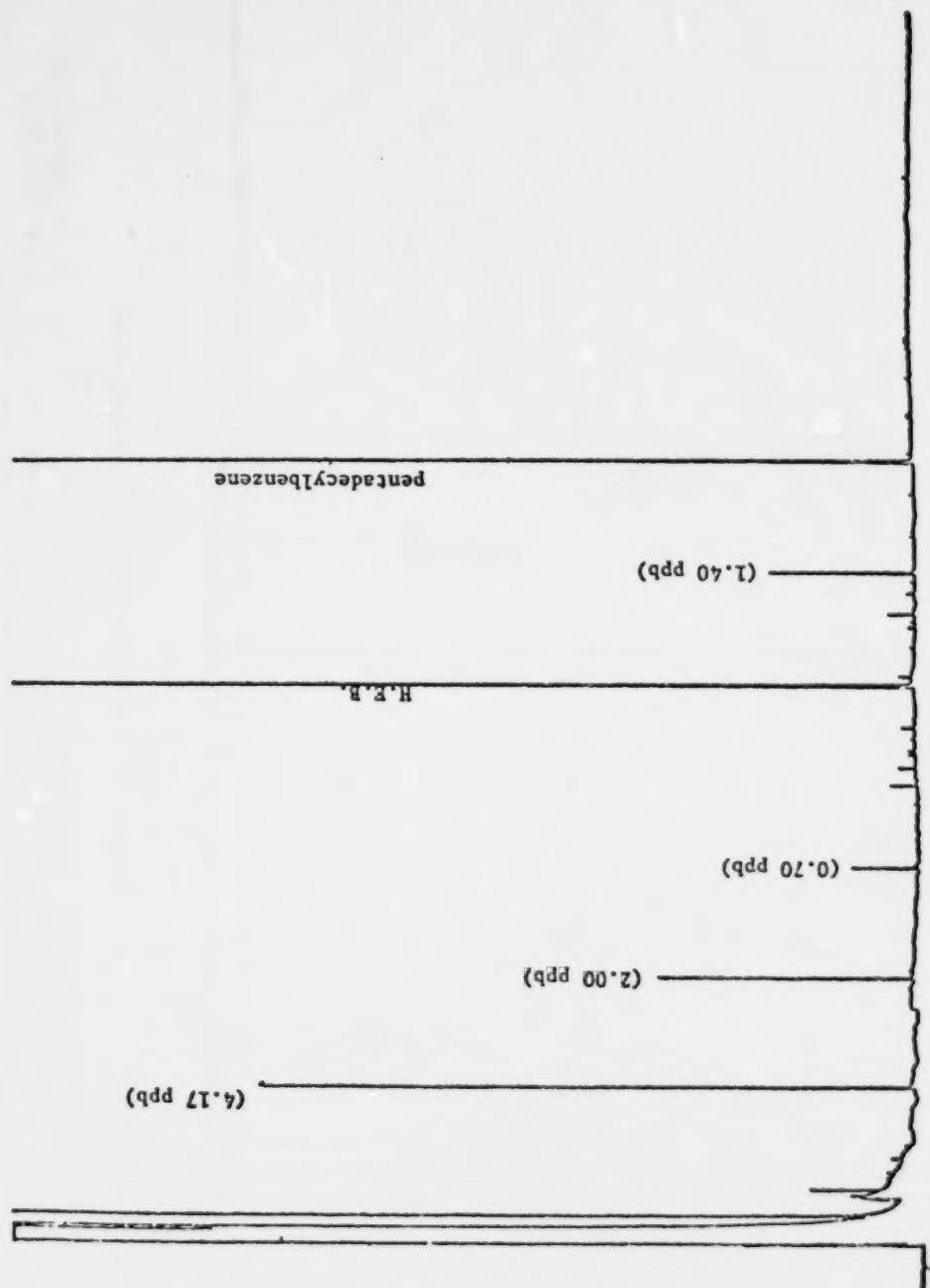


Figure 14. Basic fraction process blank

Experimental conditions: 2 μ l injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260° (held for 35 minutes).

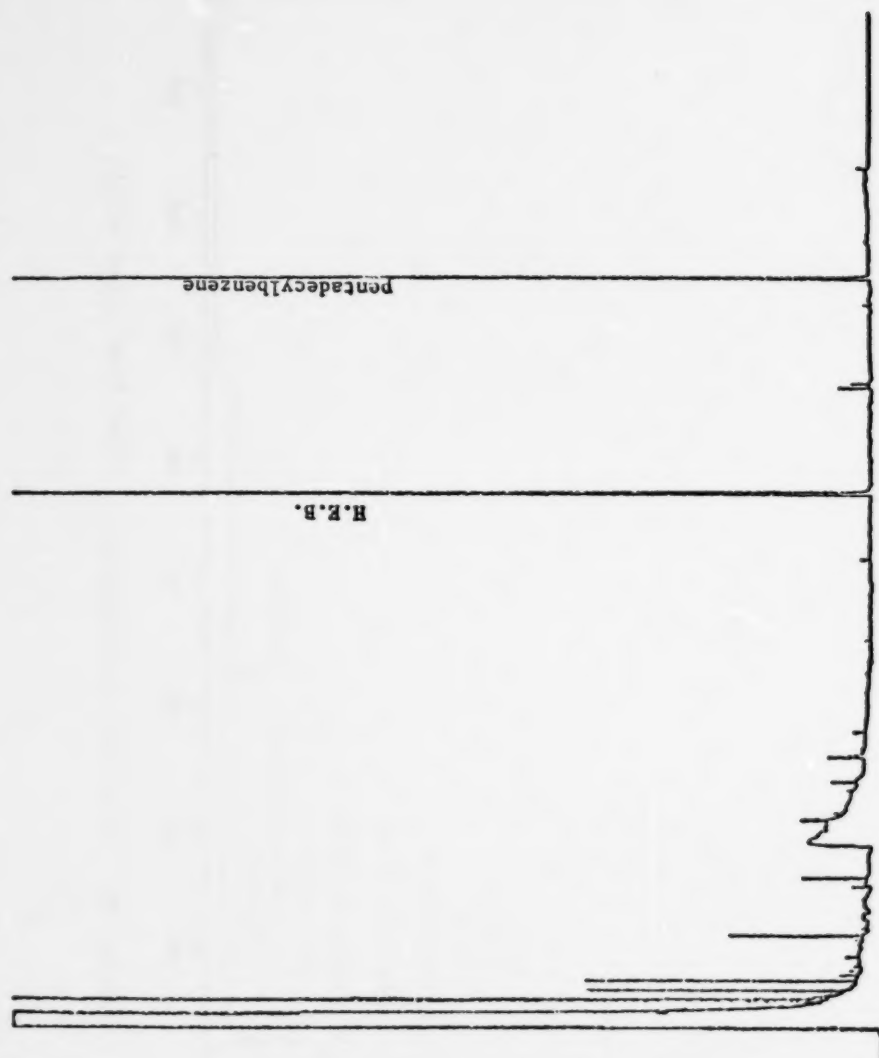


Figure 15. Acidic fraction process blank

Experimental conditions: 2 μ l injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes).

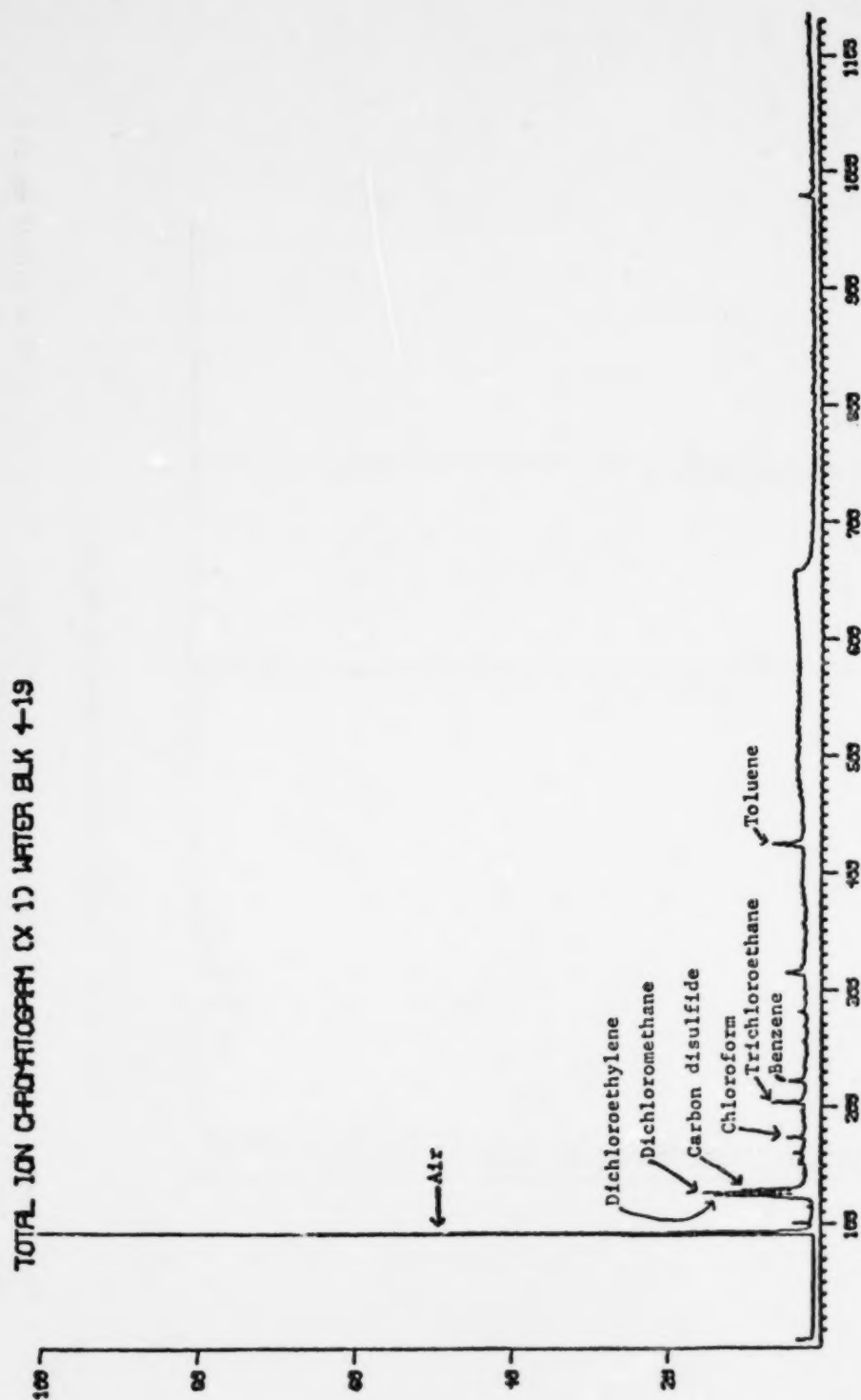


Figure 16. Total ion chromatogram obtained from water blank.

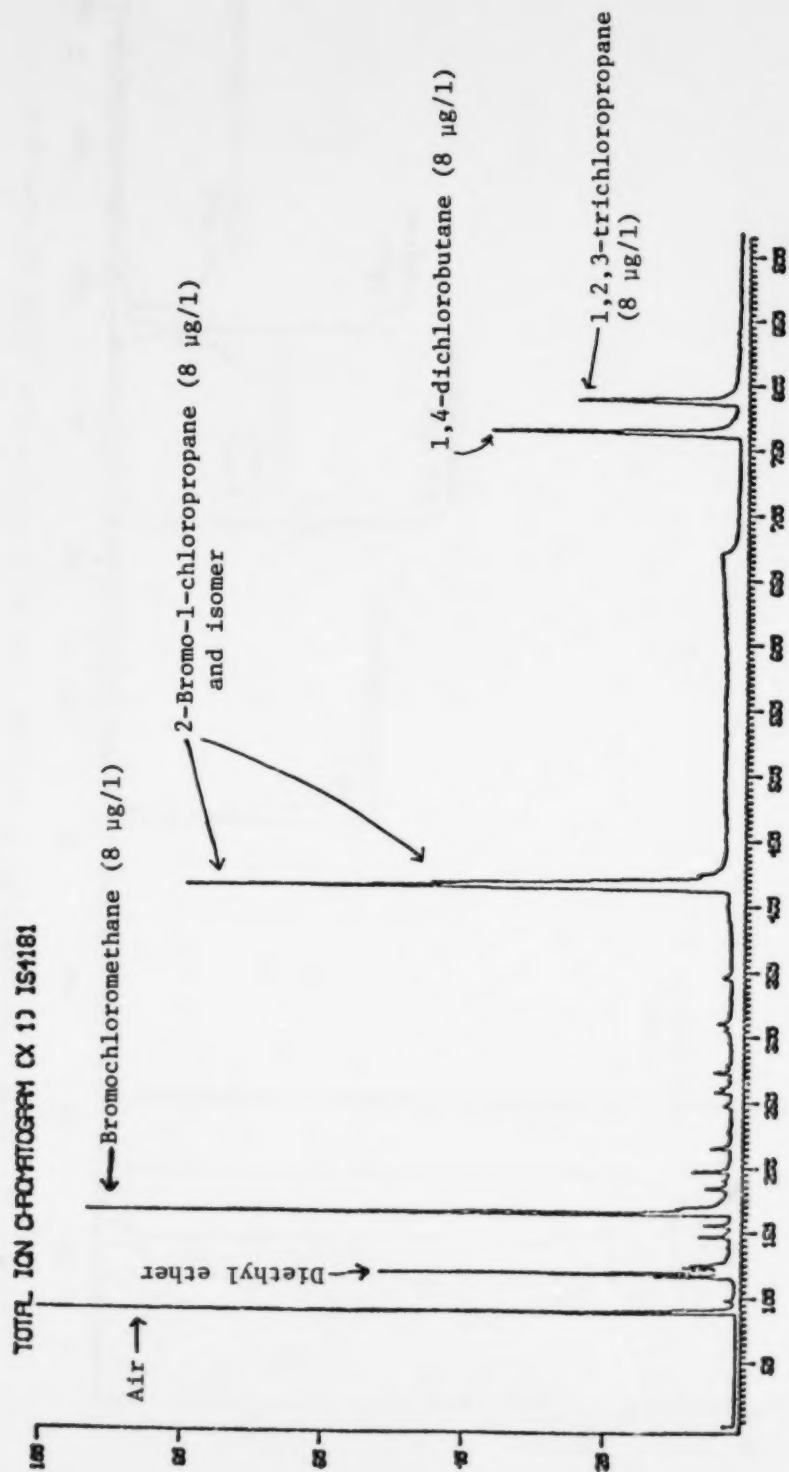


Figure 17. Total ion chromatogram obtained from water spiked with internal standards

TOTAL ION CHROMATOGRAM (X 1) INTERNAL STD4 PLUS EXTERNAL STD 4181

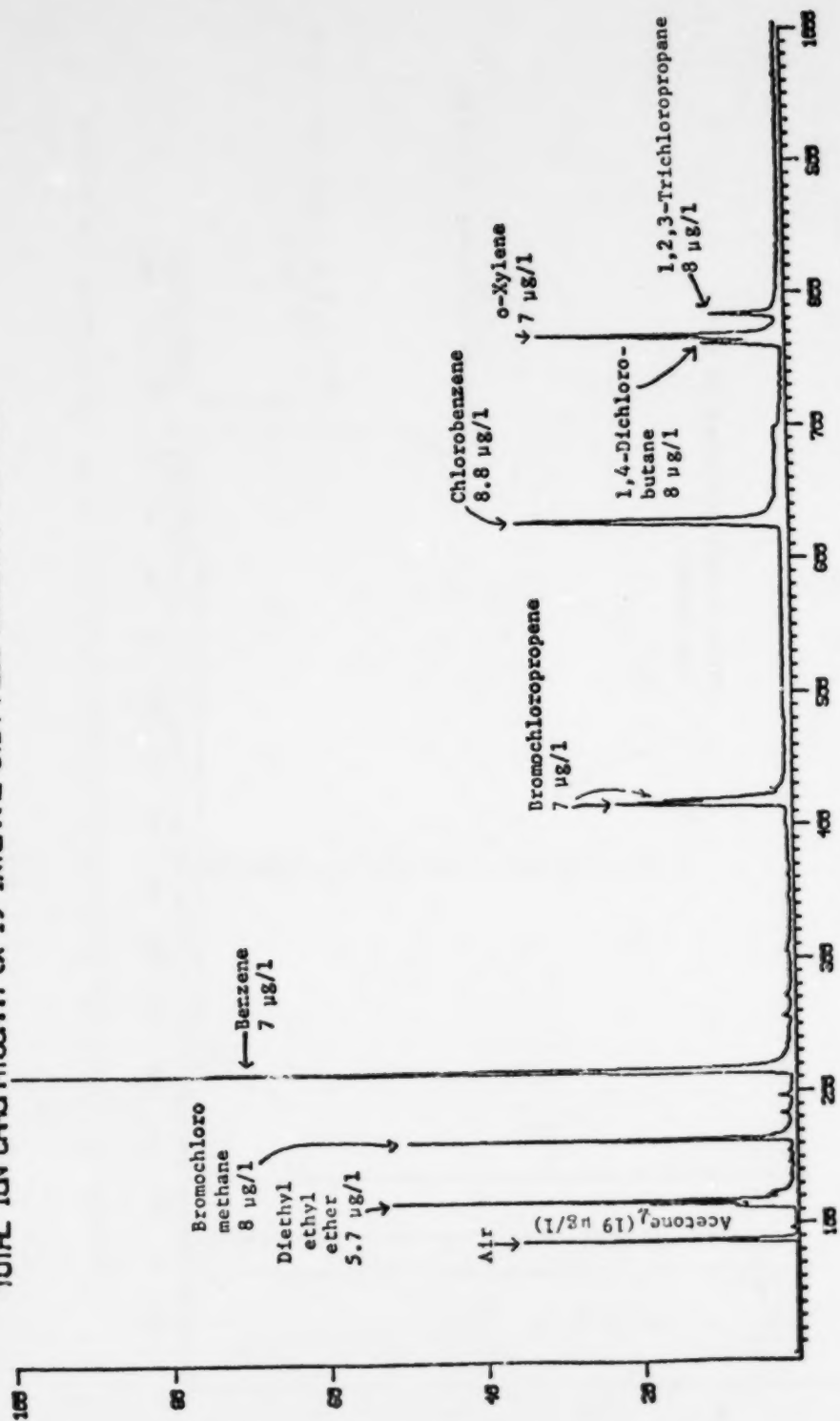


Figure 18. Total ion chromatogram obtained from water spiked with internal standards and external standards

TABLE 7. PRIORITY CRITERIA FOR GC-MS ANALYSIS

Priority	Criteria
0	A zero priority rating is given to any fraction which contains no compounds above a concentration of 4 $\mu\text{g/l}$ or contains compounds 4 $\mu\text{g/l}$ that have been tentatively identified by retention index or GC patterns in context with historical data.
+	A "+" priority rating is given to fractions on the basis of the following criteria. Compounds greater than 4 $\mu\text{g/l}$ but not sufficient for ++ priority.
++	A "++" priority rating is given to fractions on the basis of the following criteria. • 10 or more neutral compounds with conc > 10 $\mu\text{g/l}$ not previously identified • 4 or more acidic compounds with conc > 10 $\mu\text{g/l}$ not previously identified • 2 or more basic compounds with conc > 10 $\mu\text{g/l}$ not previously identified • Conc. of any given compounds > 100 $\mu\text{g/l}$.

RESULTS AND DISCUSSION

The procedures used to tentatively identify each organic compound, while specific for individual compounds, employed these general operations. First, the GC/MS/COMP analysis of each sample generated many individual mass spectra and total ion chromatograms (TIC). Inspection of each TIC resulted in the selection of a mass spectrum number and a background subtract spectrum number for each "peak" likely to produce a good mass spectrum. Second, a computerized Biemann mass spectral matching system (NIH-EPA data base, ~25,000 spectra) generated a Similarity Index (S.I.=1.000=perfect match) for the spectrum of each semivolatile compound with a concentration greater than 10 µg/l and selected volatile compounds. The S.I. provided a good first guess as to a compound's identity, but it was unreliable in determining the degree of certainty of a compound's identity. Consequently, many of the mass spectra were manually interpreted and compared to reference spectra in published data bases (2,3) before a tentative identification was made.

Samples containing many and/or concentrated components produced "mixed" mass spectra (two or more compounds eluting simultaneously) in the GC/MS analysis. In many instances of coeluting peaks only general compound names could be assigned (alkyl alcohol, subst. benzoic acid, subst. benzene). Individual isomers and/or members of a class of compounds (C₅-alkylbenzenes, fatty acid methyl esters) were rarely identified because time and funds did not permit the required analyses with authentic compounds. In general, the two limiting factors concerning the tentative identification of organic compounds were the "purity" of each sample component mass spectrum and whether or not each compound's spectrum was in accessible data bases.

TENTATIVE IDENTIFICATION OF VOLATILE COMPOUNDS

The analysis of 63 industrial effluents for purgeable organic compounds resulted in tentative identifications of 159 compounds. In general, the compounds were cleanly separated from each other resulting in clean, easily interpretable spectra. A few samples were selected for Biemann spectral matching on the computer, but most of the compounds were tentatively identified using manual interpretation procedures and the aid of published data bases.(2,3)

Table 8 is a comprehensive list of the volatile compounds tentatively identified in the 63 industrial waste-water effluents and their frequency of occurrence. The purgeable organic compounds tentatively identified in each of the 85 samples (63 effluents, 22 intakes) are listed in tables found in the Appendix.

Table 8. Volatile Compounds Tentatively
Identified in 63 Industrial Effluents

Compound (a)	Frequency of Occurrence at Given Concentration (b)			Total
	*	**	***	
<u>Hydrocarbons</u>				
Aliphatic				
Butene	8	2		10
C ₅ H ₁₀	1			1
C ₆ H ₁₄	1			1
C ₇ H ₁₄	3		1	4
C ₇ H ₁₆	2			2
C ₈ H ₁₆	5	1		6
C ₉ H ₁₈	3	1		4
C ₉ H ₂₀	2			2
C ₁₀ H ₁₂	1			1
C ₁₀ H ₁₆	1	1		2
C ₁₀ H ₂₀	1			1
Cyclohexadiene	1			1
Cyclohexane	3			3
C ₃ -Alkylcyclohexane	3			3
C ₄ -Alkylcyclohexane	3			3
Cyclohexene	1			1
Cyclooctatetraene			2	2
Cyclopentadiene		1		1
Cyclopentene	1			1
Decane	4			4
Decene	1	1		2
Diisopropylethane	4			4
Dicyclopentadiene	2			2
Dimethylbutane	9			9
Hexane	2	1		3
Heptane	1			1
Methylcyclohexane	1			1
Methylcyclopentane	9	1		10
Methylpentane	12			12
Nonane	4			4
Octane	1			1

Table 8. (Continued)

Compound (a)	Frequency of Occurrence at Given Concentration (b)			
	*	**	***	Total
Octene		1		1
Pentane		1		1
Pentene	1			1
Propene		1		1
Trimethylpentene	2			2
Tetramethylcyclopropane	2		1	3
Undecane	1			1
Vinylcyclohexene	3			3
Aromatic				
Benzene (a)	23	5	1	29
Biphenyl			1	1
C ₂ -Alkylbenzene (a, if ethylbenzene)	19	4	2	25
C ₃ -Alkylbenzene	11	6		17
C ₄ -Alkylbenzene	8	2	1	11
C ₅ -Alkylbenzene	2	1	1	4
Divinylbenzene	1			1
Ethylbenzene (a)	2			2
Indene	1			1
Methylstyrene	4	1	1	6
Naphthalene (a)	3	1		4
Styrene	1			1
C ₂ -Alkylstyrene	3		1	4
Toluene (a)	29	7	5	41
o-Xylene	3			3
m-Xylene	2			2
p-Xylene	2			2
Halo-Compounds				
Aliphatic				
Bromodichloromethane (a)	10	4		14
Bromoform (a)	2			2
Carbon tetrachloride (a)	3	3		6
Chlorobutane	1			1

Table 8. (Continued)

Compound (a)	Frequency of Occurrence at Given Concentration (b)			
	*	**	***	Total
Chlorobutene	2	1		3
Chloroethane (a)	2			2
Chloroform (a)	25	15	2	42
Chloroprene	1	1		2
Chloropropane	1			1
Chloropropene	2			2
Dibromochloromethane	6	2		8
Dibromoethane	1			1
1,1-Dibromoethane	1			1
Dibromomethane			1	1
Dichlorobutane		1		1
2,3-Dichlorobutane	1			1
Dichlorobutene		1		1
Dichlorocyclooctadiene	1			1
Dichloroethane (a)	13	2		15
Dichloroethylene (a)	18	4		22
Dichloromethane (a)	24	27	5	56
Dichloromethylenepropane	1			1
Dichloromethylpropane		1		1
Dichloropropane (a)	9	3		12
Dichloropropene	1			1
Ethyl chloride		1		1
Fluorotrichloromethane	1			1
Tetrachloroethene (a)	6			6
1,1,2,2-Tetrachloroethane (a)	4	1		5
Trichloroethane (a)	5			5
1,1,1-Trichloroethane (a)	31	5		36
Trichloroethylene (a)	11	3		14
Trichlorofluoromethane (a)	2	1		3
1,2,2-Trichloropropane	1			1
Trichlorotrifluoroethane	1			1
Aromatic				
Benzotrifluoride	1			1
Chlorobenzene (a)	2	3	1	6
Chloroethylbenzene	1			1

Table 8. (Continued)

Compound (a)	Frequency of Occurrence at Given Concentration (b)			
	*	**	***	Total
Chlorotoluene	1	1		2
Dichlorobenzene (a)	6	4	1	11
Trichlorobenzene (a)	1			1
<u>Alcohols, Aldehydes and Ketones</u>				
Aliphatic				
Acetone	5	12	10	27
2-Butene-1-ol	1			1
Butyl ketone	2			2
Butyraldehyde	1	1		2
Crotonaldehyde	1			1
Ethylbutyraldehyde	1			1
2-Ethyl-1-hexanol			1	1
Hexanone	1			1
Heptanone	2			2
Isobutyraldehyde			1	1
Isopropyl alcohol	1		2	3
Methylbutyraldehyde	1			1
Methylcyclopentanone	1			1
Methylethyl ketone	9	2		11
Methylheptanone		1		1
Methylisobutyl ketone	3			3
Methylisopropyl ketone	1			1
Methylpentanone	1	1		2
Methylpropenal	1			1
Methyl-t-butyl ketone	1			1
Nonone	1			1
2-Pentanone	1			1
3-Pentanone	2			2
<u>Ethers and Esters</u>				
Aliphatic				
Butyl acetate	1			1
Butyl ether	1			1
Di-sec-butoxyethane	1			1

Table 8. (Continued)

Compound ^(a)	Frequency of Occurrence at Given Concentration ^(b)			
	*	**	***	Total
Diethyl ether	6	2	1	9
Dihydrofuran		1		1
Diisopropyl ether	6	3	1	10
Dimethyl ether			2	2
1,4-Dioxane	1			1
2-Ethyl-1,3-dioxolane		1		1
Ethylisopropyl ether	1			1
Furan	1			1
Methyl-1,3-dioxolane		1		1
Methylethyl-1,3-dioxolane		1		1
Tetrahydrofuran	11	1	1	13
Vinyl formate	1			1
Aromatic				
Diphenyl ether			1	1
<u>Sulfur Compounds</u>				
Carbon disulfide	6	2		8
Carbonyl sulfide		1		1
Diethyl disulfide		1		1
Diethyl sulfide	1			1
Dimethyl disulfide	2	1		3
Dimethyldithiahexane		1		1
Dimethyl sulfide	2		1	3
Dimethylthiacyclopentane	1			1
Dithiahexane		1		1
Ethanethiol	1			1
Ethyl mercaptan	1			1
Ethyl-1-methylethyl disulfide	1			1
Methylethyl sulfide		1		1
Methylpropyl sulfide	1			1
Methylthiacyclohexane	1			1
Methylthiacyclopentane	1			1
Methylthiaethylbenzene	1			1

Table 8. (Continued)

Compound ^(a)	Frequency of Occurrence at Given Concentration ^(b)			
	*	**	***	Total
3-Methyl-2-thiapentane	1			1
Thiacyclopentane	1			1
<u>Miscellaneous Compounds</u>				
N-N-Dimethylformamide	1			1
Methoxytrimethylsilane		1		1
Oxazole	1			1
Trimethylsilanol			1	1

(a) Priority pollutant.

(b) Compound concentration levels: * = <10 µg/l
 ** = 10-100 µg/l
 *** = >100 µg/l

The effluent samples analyzed for purgeable components ranged in complexity from those as clean as drinking water to some that were quite smelly and containing compounds with concentrations in the mg/l range. The most polluted samples (number and amount of compounds) were from paint companies. Generally, most volatile compounds were found in the 10-100 µg/l range. The 159 compounds are classified in Table 9.

These compounds range in volatility from chloroethane (b.p. = 12.3°C) to trichlorobenzene (b.p. = 213.5°C), which was also identified in the semi-volatile fractions. In some cases, such as C₃-alkylbenzenes, many isomers of the same generic compounds were identified but were classified as one compound in Tables 8 and 9.

Twenty-two purgeable priority pollutants were identified and they occurred 359 times, 51% of the total number of occurrences of volatile compounds. Thirteen priority pollutants occurred in more than 10% of the total samples while only methylene chloride, chloroform, toluene and 1,1,1-trichloroethane occurred in more than half the samples.

TENTATIVE IDENTIFICATION OF NEUTRAL COMPOUNDS

The GC/MS analysis of 33 industrial effluents for neutral semivolatile compounds resulted in the tentative identification of 261 compounds listed in Table 10. Generally, the neutral fractions contained more compounds than either the acidic or basic fractions. Concentration levels were usually in the 10-100 µg/l range but numerous compounds were found in greater than 100 µg/l concentrations. In many cases, the large number and/or high concentration of compounds resulted in coeluting peaks. Consequently, the

TABLE 9. CLASSIFICATION OF IDENTIFIED PURGEABLE COMPOUNDS

Compound Type	Total No. Identified	Total No. of Occurrences	Priority Pollutants	
			No. Identified	No. of Occurrences
Hydrocarbons				
Aliphatic	39	115	0	0
Aromatic	17	154	4	101
Halogenated Compounds				
Aliphatic	35	271	15	240
Aromatic	6	22	3	18
Alcohols, Aldehydes & Ketones				
Aliphatic	23	68	0	0
Ethers and Esters				
Aliphatic	15	45	0	0
Aromatic	1	1	0	0
Sulfur Compounds	19	30	0	0
Miscellaneous Compounds	4	4	0	0
TOTAL	159	710	22	359

mass spectra were mixtures of two or more compounds. In many of these cases, only general identifications could be made, if at all. Tables found in the Appendix list the neutral semivolatile compounds tentatively identified in each of the 39 priority rated neutral fractions (33 effluents, 6 intakes). The 261 neutral compounds are classified in Table 11.

Hydrocarbons and halocarbons accounted for about 51% of the compounds while 30% were aromatic compounds. Alkylbenzenes, particularly C₂-alkylbenzenes, occurred the most frequently. Eleven priority pollutants were identified and occurred collectively 46 times, 10% of the 474 total occurrences of neutral compounds.

General patterns concerning the type of industry versus compounds in effluents could not be distinguished in this project due to the limited number of samples. However, some interesting compounds were found, such as: N-methyl-N-nitrosomethanaminobenzene, iodochlorocyclohexane, and substituted benzofuranones.

Table 10. Neutral compounds tentatively identified
in 33 industrial effluents

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
<u>Straight or Branched Chain Compounds</u>					
<u>Hydrocarbons</u>					
Heptane	31E			1	1
Alkane C $\geq$ 8	31E	1	1		2
Alkane C $\geq$ 9	31E	2	1	1	4
Decane	54E	2	3		5
Branched Hydrocarbon	1E		1		1
Undecane	54E	4	1		5
Alkane C $\geq$ 11	12E	1	1		2
Dodecane	26E	1	1		2
Alkane C $\geq$ 12	12E	1		1	2
Tridecane	54E	1	1		2
Alkane C $\geq$ 13	54E	2	1	1	4
Tetradecane	29E	1		2	3
Alkane C $\geq$ 14	29E	2	1	1	4
Pentadecane	29E	1	2	1	4
Alkane C $\geq$ 15	54E		1		1
Hexadecane	54E	1	1	2	4
Alkane C $\geq$ 16	25E		2	1	3
Heptadecane	29E	3	2	1	6
Alkane C $\geq$ 17	54E	2		1	3
Octadecane	25E		1	1	2
Alkane C $\geq$ 18	29E		2		2
Nonadecane	25E	1	3		4
Alkane C $\geq$ 19	26E		2		2
Eicosane	4E	1	2		3
Heneicosane	26E	1	3		4
Alkane C $\geq$ 21	29E	1	1		2
Docosane	26E		1		1
Tricosane	26E		1		1
Branched Hydrocarbon C $\geq$ 23	1E	1			1
Tetracosane	1E		1		1

Table 10. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
Alkane C $\geq$ 24	58E		1		1
Pentacosane	40E		2		2
Alkane C $\geq$ 25	26E		1		1
Hexacosane	26E		1		1
Heptacosane	26E		2		2
Octacosane	26E		1		1
Nonacosane	26E		1		1
Nonene	33E		1		1
Methyloctene	29E		1		1
Decene	29E			1	1
Methylnonene	33E		1		1
Alkene C $\geq$ 11	25E	1			1
Dodecene	29E			1	1
Alkene C $\geq$ 12	31E	1	1		2
Alkene C $\geq$ 13	26E			1	1
Tetradecene	29E			2	2
1-Propene-2-methyl trimer	34E		1		1
Alkene C $\geq$ 15	29E		1		1
Hexadecene	29E			1	1
Alkene C $\geq$ 17	29E			1	1
Octadecene	29E		1		1
Alkene C $\geq$ 19	29E		1		1
Eicosene	29E		1		1
1-Propene-2-methyl tetramer	34E		1		1
Alkene C $\geq$ 20	29E		1		1
Alkene C $\geq$ 22	29E		1		1
Alkene C $\geq$ 23	29E		1		1
Alkene C $\geq$ 27	29E		1		1
Alkene C $\geq$ 29	29E		1		1
Dimethyldecene	29E			1	1

Table 10. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
Halocarbons					
1,3-Butadiene,2-chloro-dimer	34E			1	1
C ₄ H ₆ Cl ₂	45E			1	1
Chloroalkene	45E			1	1
Chlorohydrocarbon	58E	1			1
Dichlorobutene	45E		1		1
Dichloropropene	35E		1		1
Halo-alkane	4E	1			1
Halo-alkene	21E		1		1
Iodoheptane	49E			1	1
Tetrachloroethane	60E	1			1
Alcohols					
Alkyl alcohol	31E		5		5
Alkyl alcohol C $\geq$ 8	31E		1		1
Alkyl alcohol C $\geq$ 9	22E		3		3
Alkyl alcohol C $\geq$ 11	25E	1	1		2
Alkyl alcohol C $\geq$ 12	22E	1	2	1	4
Dimethylpentanol	35E		1	1	2
Docosanol	29E		1		1
Eicosanol	8E	1			1
Heptadecanol	35E		1		1
Hexenol	21E			1	1
Methylheptanol	31E			1	1
Octanol	29E		1		1
Propylheptanol	29E			1	1

Table 10. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
Ethers					
Alkyl ether	33E		2		2
Alkenyl ether	33E		1		1
2-Butoxyethanol	30E	1	4		5
n-Butyl ether	7E	1			1
Ethanol,2-(1-(2-butoxy ethoxy)	7E	1			1
Ethanol,1-(2-butoxy ethoxy)	45E			1	1
Hexoxy butanol	15E	1			1
2-Propanol,1-(2-methoxy-1-1 methyl ethoxy)	50E		1		1
2-Propanol,1-(2-methoxy-1-1 methyl ethoxy)-isomer	50E		1		1
Ketones					
Alkyl diketone	7E	1			1
Alkyl ketone C $\geq$ 7	22E	1	1		2
Alkyl ketone C $\geq$ 10	34E		1		1
Alkyl ketone C $\geq$ 11	22E		1		1
Alkyl ketone C $\geq$ 27	22E		1		1
Dimethylpentanone	28E		2		2
Heptanone	6E	2			2
Isophorone	7E	2			2
Methyl hexanone	22E			1	1
Methyl pentanone	45E	1			1
4-Octanone	8E	1			1
Aldehydes					
Aldehyde C ₈ H ₁₆ O	35E		1		1
Methylpentanal	21E	1			1

Table 10. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
Esters					
Acetic acid C $\geq$ 8 ester	34E		1		1
Acetic acid C $\geq$ 9 ester	34E		1		1
Butyl acetate	26E			1	1
Propanoic acid-2-methyl propyl	28E		1		1
Cyclic Nonaromatic Compounds					
Hydrocarbons					
Alkylcyclohexane	9E	2			2
Alkylcyclohexene	49E		1		1
1,1'-Bicyclohexyl, ethyl	49E		1		1
Methylcyclohexane	49E	1		1	2
Halocarbons					
Bromochlorocyclohexane	21E	2	3	2	7
Chlorocyclohexane	49E	1			1
Chlorocyclohexene	15E	1	4		5
1-Chloro-5-(1-chloroethenyl) cyclohexene	34E		1		1
Dibromocyclohexane	5E	4			4
Dibromocyclohexene	15E	1			1
Dichlorocyclohexane	15E		1	3	4
Halo-cyclohexane	77E	1			1
Iodochlorlcyclohexane	49E			1	1
Subst. iodocyclohexane	49E	1			1
Alcohols					
Bromocyclohexanol	15E	2	4	1	7
C ₄ -Alkylcyclohexanol	22E		2		2

Table 10. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
Chlorocyclohexanol	15E	2	4	2	8
Cyclohexenol	15E		2		2
Methylcyclohexanol	22E		1		1
Ethers					
Bromomethoxycyclohexane	15E		2		2
Oxybisyclo[4,1,0]heptane	15E		1		1
Ketones					
Alkylcyclohexanone	33E		1		1
C ₃ -Cyclohexadienone	33E		1		1
C ₃ -Cyclohexenone	33E		1		1
Chlorocyclohexanone	9E	1			1
Methylcyclohexanone	22E		1		1
Methylcyclohexenone	35E	1	1		2
Esters					
Subst. cyclohexene carboxylic acid methyl ester	40		1		1
Aromatic Compounds					
Hydrocarbons					
Alkyl benzene	7E	3			3
Alkyl indene	33E		1		1
Alkyl naphthalene	12E	2	1		3
Alkyl tetrahydronaphthalene	45E			1	1
1,1'-Biphenyl	14E	1	3	3	7
C ₃ -Alkylbenzene	26E	1	6	2	9
C ₄ -Alkylbenzene	26E	1	3	1	5
C ₅ -Alkylbenzene	25E	1	1	2	4
C ₆ -Alkylbenzene	35E		1		1

Table 10. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
C ₂ -1,1'-Biphenyl	25E		1		1
C ₂ -Alkyldihydroindene	4E	1			1
C ₂ -Alkyldihydronaphthalene	12E	1			1
C ₂ -Alkylstyrene	35E		2		2
C ₃ -Alkynylbenzene	35E		1		1
C ₃ -Alkylstyrene	25E		2		2
C ₂ -Phenanthrene	1E	1			1
C ₃ -Phenanthrene	1E	1			1
Dihydrodimethylindene	32E		1		1
Dihydronaphthalene	60E		3		3
Dimethylnaphthalene	54E			1	1
Ethylbenzene (a)	26E	2	6	2	10
Ethylstyrene	30E	1	1		2
Indene	32E		1		1
1H-Indene-1-ethyl-2,3-dihydro	25E		1		1
Methyl-1,1'-biphenyl	25E	1			1
Methylindene	32E		2		2
Methylnaphthalene	26E		4	1	5
Methyl phenanthrene	1E	1			1
Methylstyrene	26E		2		2
Methyltetrahydronaphthalene	35E		1		1
Naphthalene(a)	26E	3	3	1	7
Styrene	31E			1	1
Subst.-alkylbenzene	32E		1		1
Subst.-benzene	31E		1		1
Subst.-benzene isomer	31E			1	1
Subst. styrene	31E		1		1
Tetrahydrodimethylnaphthalene	32E		1		1
1,2,3,4-Tetrahydronaphthalene	7E		1		1
Toluene (a)	14E	2	6		8
Xylene	28E	1	5	2	8

Table 10. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
Halocarbons					
Bromonaphthalene	49E	1			1
Chlorobenzene(a)	49E	2	2		4
Chloromethylbenzene	60E	1			1
1,2-Dichlorobenzene(a)	7E		2		2
1,3-Dichlorobenzene(a)	7E	1			1
1,4-Dichlorobenzene(a)	7E	1			1
Dichloromethylbenzene	60E		1		1
Tetrachlorobenzene	60E	1			1
1,2,4-Trichlorobenzene (a)	60E		1		1
Tribromoethylbenzene		1			1
Alcohols					
Tetrahydromethylnaphthalenol	12E	1			1
Ethylbenzenemethanol	6E	1			1
1-Methyl-1-phenylethanol	28E		1	2	3
1,4-Methanonaphthalen-9-ol,1,4-dihydro	14E	1			1
1-Phenylpropanol	15E	1	1		2
Tetrahydromethylnaphthalenol	12E	1			1
Ethers					
Benzene,1,1'-Oxybis(4-methyl)	45E			1	1
1,1'-Biphenyl,2-phenoxy	7E	1			1
Diphenyl ether	28E	2		3	5
Methoxy-C ₃ -benzene	29E			1	1

Table 10. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
Ketones					
Acetophenone	45E	2	1		3
Alkylaromatic ketone	8E	1			1
Alkyl-naphthalenone	4E	1			1
Dihydroindenone	35E	1	2	1	4
Dihydro-1H-Inden-1-one	35E		1		1
o-Methoxypropylphenone	45E		1		1
1-Phenylpropanone	15E	1	1	1	3
2-Propanone,4-methyl-4-phenyl	7E	1			1
1,2,3,4-Tetrahydronaphthalen-1-one	7E		1		1
Aldehydes					
Benzaldehyde	9E	1		1	2
Ethanone,1-[4-(1-methylethyl)phenyl	25E		1		1
Ethanone,1-(2,4-dimethylphenyl)	4E	1			1
Esters					
Benzoic acid,2-propenyl ester	45E		1		1
Benzene methanol, methoxy acetate	58E		1		1
Bis(2-ethylhexyl) phthalate (a)	50E	2	1		3
Butylbenzyl phthalate(a)	26E	1	2		3
Di-2-propenyl phthalate	45E			1	1
Dibutyl phthalate (a)	14E	5	1		6
Diethyl phthalate	40E	1	1		2
Phthalate	45E	5			5
Sulfur Compounds					
Benzene-1,1'-sulfonyl bis-	63E	1			1
Benzene,1,1'-sulfonyl bis[4-chloro-]	63E			1	1

Table 10. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
N-Dimethylbenzene sulfonamide	14E	1			1
2,3-Dithiahexane	25E		1		1
3,4-Dithiahexane	25E		1		1
Methyl,4-chlorophenyl sulfone	63E	1			1
Methyldithiahexane	25E		1		1
Nonanethiol	33E		1		1
<u>Nitrogen Compounds</u>					
Benzene methanamino,N-methyl, N-nitroso	50E			1	1
N,N-Dimethylacetamide	14E	1			1
Nitroaniline	50E		1		1
Nitrobenzene	51E			1	1
Nitrocyclohexene	51E		1		1
<u>Phosphorus Compounds</u>					
Phosphordithioic acid, O,O- dimethyl-S-ethyl ester	45E		1		1
Subst. Phosphate	7E	1			1
Trialkylphenyl phosphate	7E		1		1
Tributyl phosphate	5E	1	1		2
Tricresyl phosphate	7E		1		1
Triphenylester, phosphoric acid	7E		1		1
Trixylyl phosphate	7E		1		1
Trioctyl phosphate	1E	1			1
<u>Silicon Compounds</u>					
Silicone		2	1		3
<u>Heterocyclic Compounds</u>					
Alkylphenol C _{> 15}	22E		1		1

Table 10. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
3(2H)Benzofuranone, Dimethyl	45E		1		1
3(2H)Benzofuranone, Methyl	25E		3		3
1,2,3-Benzothiadiazole	12E			1	1
Dibenzofuran	14E	1			1
Dihydromethylfuranone	60E	1			1
Dimethylbenzofuran	35E		1		1
1,3-Dioxolane,2-(chloromethyl)	50E		1		1
Methylbenzothiazole	60E	1			1
2-Propenal-3(2-furanyl)	45E		1		1
1,2-Benzisothiazol,3-ethoxy,1,1-dioxide	45E		1		1
Tetrahydrothiaphene,1,1-dioxide	32E			1	1
Subst. benzofuranone	45E			1	1
<u>Miscellaneous Compounds</u>					
Alkylphenol C $\geq$ 15	22E		1		1
Alkylphenol C $\geq$ 16	22E		1		1
2,4-Bis(1-methylethyl) phenol	7E		1		1
2,4-Bis(1-methylbutyl)phenol	50E		1		1
2,4-Bis(1-methylethyl) phenol	7E		1		1
C ₄ -Alkylphenol	45E			1	1
C ₈ -N,N-Subst. aniline	29E		1		1
Chloroalkyl subst. phenol	50E		1		1
Subst. phenol	7E	1			1

(a) Priority pollutant

(b) Representative sample in which compound was identified (see Appendix A)

(c) Compound Concentration Levels: * = <10 $\mu\text{g/l}$
 ** = 10-100 $\mu\text{g/l}$
 *** = >100 $\mu\text{g/l}$

Table 11. Classification of Compounds Identified in Neutral Fractions

Compound Type	Total No. Identified	Total No. of Occurrences	Priority Pollutants	
			No. Identified	No. of Occurrences
Straight or Branched				
Chain Compounds				
Hydrocarbons	60	115	0	0
Halogenated compounds	10	10	0	0
Alcohols	13	24	0	0
Ethers	9	14	0	0
Ketones	11	15	0	0
Aldehydes	2	2	0	0
Esters	4	4	0	0
Cyclic Non-aromatic Compounds				
Hydrocarbons	4	6	0	0
Halogenated compounds	10	26	0	0
Alcohols	5	20	0	0
Ethers	2	3	0	0
Ketones	6	7	0	0
Esters	1	1	0	0
Aromatic Compounds				
Hydrocarbons	40	105	3	25
Halocarbons	10	14	5	9
Alcohols	6	9	0	0
Ethers	4	8	0	0
Ketones	9	16	0	0
Aldehydes	3	4	0	0
Esters	8	22	3	12
Sulfur Compounds	8	8	0	0
Nitrogen Compounds	5	5	0	0
Phosphorous Compounds	8	9	0	0
Silicon Compounds	1	3	0	0
Heterocyclic Compounds	13	15	0	0
Miscellaneous Compounds	9	9	0	0
TOTAL	261	474	11	46

Table 12. Acidic Compounds Tentatively Identified
in 26 Industrial Effluents

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
<u>Aliphatic Acids</u>					
Alkenoic Acid C $\geq$ 18	9E	1			1
Alkenoic acid (branched)			1		1
Acetoxyhexanoic acid	35E		1		1
Benzeneacetic acid	53E		3		3
Benzenepropanoic acid	53E		1		1
C ₃ -Alkylphenylpropanoic acid	35E		1		1
Dimethylbutanoic acid	35E	1			1
Dimethylphenylpropanoic acid	35E		1		1
Fatty acids					
3-Methylpentanoic acid	35E		2		2
Hexanoic acid	62E		1		1
C $\geq$ 6	31E	1	7	1	9
Heptanoic acid	26E		1		1
C $\geq$ 7	31E	3	3	1	7
Octanoic acid	26E		3		3
C $\geq$ 8	31E	2	1	2	5
Nonanoic acid	26E		1		1
C $\geq$ 9	31E	1	1	1	3
Decanoic acid	26E		1		1
C $\geq$ 10	31E	2	2		4
Dodecanoic acid	26E	3	4		7
C $\geq$ 11	29E		1		1
C $\geq$ 12	43E	2			2
C $\geq$ 13	62E	1			1
Tetradecanoic acid	26E	6	5		11
C $\geq$ 14	35E	2	3		5
Pentadecanoic acid	53E	2	1		3

Table 12. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
C $\geq$ 15	18E	5	3		8
Hexadecanoic acid	29E		7	2	9
C $\geq$ 16	18E	3	4		7
Heptadecanoic acid	56E	1			1
C $\geq$ 17	56E	4	3		7
Octadecanoic acid	26E	5	3		8
C $\geq$ 18	31E	5	5	1	11
C $\geq$ 19	53E	1			1
Eicosanoic acid	9E	1			1
C $\geq$ 20	40E	1	2		3
C $\geq$ 21	40E	1	1		2
C $\geq$ 22	40E	1	1		2
C $\geq$ 23	40E		1		1
C $\geq$ 24	40E		1		1
Methylcyclohexene-1-carboxylic acid	22E		2		2
Methylphenylpropanoic acid	35E		1		1
Octadecadienoic acid	26E	1	2	1	4
Octadecenoic acid	26E	2	2	2	6
Subst. cyclohexane acid	2E	1			1
<u>Aromatic Acids</u>					
Alkylbenzoic acid	35E		2		2
Benzenedicarboxylic acid	50E		1		1
Benzoic acid	28E	2	8	1	11
C ₅ -Alkyloctahydrophenanthrene carboxylic acid	58E		2		2
Dimethylbenzoic acid	35E		1		1
Ethenylbenzoic acid	35E		1		1
Methylbenzoic acid	26E		3		3
Octahydro-1,4-dimethyl-1-(methylethyl)phenanthrene carboxylic acid	52E		1		1

Table 12. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
Octahydrodimethylphenanthrene carboxylic acid	22E		1		1
Subst. phenanthrene carboxylic acid	31E		3		3
Subst. benzoic acid	12E	1	1		2
Trimethylbenzoic acid	26E		2		2
<u>Haloaliphatic Acids</u>					
Chloro-fatty acid	9E	1			1
Halo-acid	9E	1			1
<u>Haloaromatic Acids</u>					
Chlorobenzoic acid	60E		2		2
Chloroalkylbenzoic acid	12E	1			1
Dichlorobenzoic acid	60E	2			2
<u>Alkylphenols</u>					
Alkylphenol	34E		1		1
Benzene[(dihydroxy)methyl]	58E	1			1
Benzene,1-hydroxy-2-[(4-hydroxyphenyl)]	58E	1			1
C ₂ -Alkylphenol	44E			1	1
C ₃ -Alkylphenol	44E		1		1
C ₄ -Alkylphenol	44E	1	2		3
C ₄ -Alkenylphenol	44E		1		1
Dimethylphenol(a)	43E		4		4
Isomer of phenol 2-[(4-hydroxyphenyl)methyl]	58E	1			1

Table 12. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			
		*	**	***	TOTAL
Methylallylphenol	44E		1		1
Methylphenol	29E	1	5	3	9
Nonylphenol	22E		1		1
Phenol(a)	60E		5	7	12
Phenol,2,6-[4-(hydroxyphenyl)dimethyl]	52E		2		2
Phenol,2-[4-(hydroxyphenyl)methyl]	52E		1	1	2
<u>Halophenols</u>					
Bromomethylphenol	53E		3		3
Bromophenol	52E	1	4		5
Chloroalkylphenol	58E	1			1
Chlorobromosubst.-phenol	58E	1			1
Chlorophenol(a)	52E		3	4	7
Chloromethylphenol(a)	57E	1	2		3
Dichlorophenol(a)	58E		3		3
Trichlorophenol(a)	50E	1	2		3
<u>Benzenesulfonic Acid Derivatives</u>					
Benzenesulfonic acid-4-hydrocyhydrazide	34E		1		1
Benzenesulfonamide,N,4-dimethyl	52E	2	2		4
p-Toluenesulfonamide	9E		3		3
Subst.-benzenesulfonic acid	34E		1		1
<u>Heterocyclic Compounds</u>					
Benzothiadiazole	12E	1			1
Methoxy-1,2-benzothiazole	60E		1		1
Methoxythiobenzothiazole	60E		1		1
Subst.-benzisothiazole	60E	1			1

Table 12. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
<u>Miscellaneous Compounds</u>					
Allylthiopropanoic acid	35E	1			1
Dihydroxybenzaldehyde	58E	1			1
Dimethylhydroxybenaldehyde	18E		1		1
Hydroxybenzoic acid	32E	2			2
Hydroxybenzeneacetic acid	50E	1			1
Hydroxytrimethylbenzoic acid	50E	1			1
Hydroxymethylbenzoic acid	35E		1		1
Indolinecarboraldehyde, hydroxymethyl	18E		1		1
Oxiraneoctanoic acid,2-octyl	9E		1		1
Octadecanoic acid,9,10-dihydroxy	9E		1		1
Thienopyridine	60E		1		1

(a) Priority Pollutant

(b) Representative sample in which compound was identified (see Appendix A)

(c) Compound Concentration Levels: * = <10 µg/l
 ** = 10-100 µg/l
 *** = >100 µg/l

TENTATIVE IDENTIFICATION OF ACIDIC COMPOUNDS

The GC/MS analysis of 26 industrial effluents for acidic semivolatile compounds resulted in the tentative identification of 104 compounds. The compounds listed in Table 12 are names as the parent compound, although methylation with diazomethane meant that certain acidic compounds were actually identified as methyl esters and/or methyl ethers.

Because mass spectra of many of these methylated compounds were not included in accessible data bases the number of tentative identifications in the acidic fractions was limited. Tables in the Appendix list the acidic semivolatile compounds tentatively identified in each of the 29 priority rated acidic fractions (26 effluents, 3 intakes).

The acidic fractions of the 26 effluent samples analyzed were generally less complex than the neutral fractions but contained more components than the basic fractions. Most acidic compounds were found with concentrations

of 10-100 $\mu\text{g/l}$. No particular type of company had effluents which could be distinguished from one another on the basis of their acidic compound content (concentration and number of compounds). The 104 acidic compounds are classified in Table 13.

Not surprisingly, aliphatic acids were the most numerous compounds followed by alkylphenols and aromatic acids. Six priority pollutants were identified - phenol (12 times), chlorophenol (7 times), dichlorophenol (3 times), trichlorophenol (3 times), dimethylphenol (4 times) and chloromethylphenol (3 times). Fifty-six compounds occurred only once, while phenol and benzoic acid occurred 12 and 11 times respectively. The acidic compounds occurred a total of 272 times while priority pollutants accounted for only 32 occurrences, about 12% of the total number of occurrences.

TENTATIVE IDENTIFICATION OF BASIC COMPOUNDS

The analysis of 21 industrial effluents for basic semivolatile compounds resulted in the tentative identification of 49 compounds listed in Table 14. Tables found in the Appendix list the basic compounds tentatively identified in each of the 21 effluent samples.

TABLE 13. CLASSIFICATION OF COMPOUNDS IDENTIFIED IN ACID FRACTIONS

Compound Type	Total No. Identified	Total No. of Occurrences	Priority Pollutants	
			No. Identified	No. of Occurrences
Aliphatic acids	45	143	0	0
Aromatic acids	12	30	0	0
Halo-aliphatic acids	2	2	0	0
Halo-aromatic acids	3	5	0	0
Alkylphenols	15	41	2	16
Halophenols	8	26	4	16
Benzenesulfonic acid derivatives	4	9	0	0
Heterocyclic compounds	4	4	0	0
Miscellaneous compounds	11	12	0	0
TOTAL	104	272	6	32

Generally, the basic compounds found in the effluent samples were present in smaller numbers and lower concentration ($<10 \mu\text{g/l}$) compared to the neutral and acidic compounds. Steel companies, as a group, had effluents with the highest number of basic compounds, and in some cases, the basic compounds were the most concentrated components in the sample. It should be noted that all the basic compounds present in the effluent extracts probably did not elute from the SE-30 capillary column. This result was expected--future analyses should use a more suitable column for basic components. The 49 basic compounds are classified in Table 15.

The basic compounds occurred a total of 70 times while no priority pollutants were identified. Methyl pyridine occurred most frequently (8 times) while 39 of the 49 compounds occurred only once. The heterocyclic compounds would appear to be the most interesting group of compounds both in biological activity and environmental significance.

SUMMARY OF IDENTIFIED COMPOUNDS IN INDUSTRIAL EFFLUENT SURVEY

During the course of this industrial effluent survey many different types of data have been generated. Correlation of these different data types can be done in a number of ways depending upon one's perspective and interests. Table 16 correlates the number of identified compounds with various other parameters. This representation may be useful in determining the environmental significance of compounds found in industrial effluents.

Table 14. Basic Compounds Tentatively Identified
in 21 Industrial Effluents

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
<u>Aliphatic Amines</u>					
Alkyl amine	22E	1	1		2
Cyclohexyl amine	52E			1	1
Hexamethylenetetramine	56E		1		1
N-Butyl-1-butamine	62E			1	1
N-Butyl,N-methyl-1-butamine	62E	1	1		2
N-Phenylmethylenheptamine	22E	1			1
<u>Aromatic Amines</u>					
Diethylaniline	29E		1		1
Dimethylaniline	30E	2	3		5
Methylaniline	50E	1	1	1	3
N-Ethyl-o-toluidine	29E	1			1
N,N-Diethylaniline	54E	1			1
Pentamethylaminobenzene	45E		1		1
<u>Heterocyclic Compounds</u>					
Alkylaziridine (C ₈ H ₁₇ N)	22E			1	1
Benzo[c]methylcinnoline	18E		1		1
C ₃ -Alkylpyridine	54E	2			2
C ₄ -Alkylpiperidine	45E		1		1
C ₄ -Alkylpyridine	33E	2	1		3
C ₅ -Alkylpyridine	33E		1		1
C ₅ -Alkylquinoline	34E	1			1

Table 14. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
C ₃ -Benzimidazole	18E		1		1
Dimethylbenzimidazole	18E		1		1
2,6-Dimethyl-4-ethylpyridine	33E		1		1
Dimethylnaphthyridine	18E	1			1
Dimethylquinoline	32E	1			1
Imidazolidine, C ₂ -alkylphenyl	49E	1			1
Imidazolidine, C ₃ -alkylphenyl	49E	1			1
Isoquinoline	18E		1		1
Methylbenzimidazole	18E		1		1
3-Methylcinnoline	18E		2		2
Methylisoquinoline	18E		1		1
Methylnaphthyridine	18E		1		1
Methylpyridine	18E		5	3	8
1,6-Naphthrydine	18E		1		1
Phenanthroline	18E		1		1
Phenothiazine	34E		1		1
Pyridine, 3-(1-Methyl-2-pyrrolidinyl)	54E	1			1
Pyrrolo(2,3,8-pyridine, dimethyl	18E		1		1
Quinoline	53E	1	1		2
Trimethylpiperidine	45E		1		1
Trimethylpyridine (2 isomers)	33E			1	1
<u>Miscellaneous Compounds</u>					
Cyanopyridine	22E		1		1
2-Diethylaminoethanol	52E			1	1
5-Hexen-3yn-2-one, 6-(1-piperidinyl)	52E		1		1
Hydroxymethylimidazole	52E			1	1

Table 14. (Continued)

COMPOUND ^a	SAMPLE NO. ^b	Frequency of Occurrence at Given Concentration ^c			TOTAL
		*	**	***	
2-Methoxyaniline	50E			1	1
Methoxyaniline	45E		2		2
3-Methyl-5-ethoxypyrazole	50E		1		1
2-Propen-1-amine, N,N-di-2-propenyl	34E		1		1
1,3,5-Triazine-2,4-diamine, 6-(3-methyl-phenyl)	34E	1			1

(a) Priority Pollutant

(b) Representative sample in which compound was identified (see Appendix A)

(c) Compound concentration levels:

* = <10 µg/l

** = 10-100 µg/l

*** = >100 µg/l

TABLE 15. CLASSIFICATION OF COMPOUNDS IDENTIFIED IN BASIC FRACTIONS

Compound Type	Total No. Identified	Total No. of Occurrences	Priority Pollutants	
			No. Identified	No. of Occurrences
Aliphatic amines	6	8	0	0
Aromatic amines	6	12	0	0
Heterocyclic compounds	28	40	0	0
Miscellaneous compounds	9	10	0	0
TOTAL	49	70	0	0

TABLE 16. SUMMARY OF IDENTIFIED COMPOUNDS IN INDUSTRIAL EFFLUENT SURVEY

Sample Type	No. of Effluents Analyzed	No. of Compounds Identified	Total No. of Occurrences	No. Found in Only One Effluent	Priority Pollutants	
					No. Identified	Total No. of Occurrences
Purged Effluent	63	159	710	85	22	359
Extract-neutral fraction	33	261	474	176	11	46
Extract-acid fraction	26	104	272	56	6	32
Extract-basic fraction	21	49	70	39	0	0
TOTAL		573 ^(a)	1526	356	39 ^(b)	437

(a) Because some purged compounds were also present in extracts, less than 573 different compounds were identified.

(b) Toluene, ethylbenzene, chlorobenzene, dichlorobenzene trichlorobenzene, and naphthalene were found in both purgeable and neutral fractions. A total of 33 different priority pollutants were identified in this survey.

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APPENDIX

SAMPLE DATA TABLES

TABLE A-1. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 1VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Testative Identification	Characteristic Ions in Mass Spectrum
1	0.16		Air	44(100)
2	0.18	<1	Butane or Methylpropane	41(100) 56(50)
3	0.20	1-10	Acetone	43(100) 58(40)
4	0.20	<1	Dichloroethylene	61(100) 96(80) 98(55)
5	0.21	1-10	Dichloromethane	49(100) 51(33) 84(85) 86(55)
6	0.21	<1	Carbon Disulfide	78(100) 80(4)
7	0.24	10-100	Butyraldehyde	44(100) 43(85) 72(55) 41(32) 57(30)
8	0.26	1-10	Chloroform	81(100) 85(66)
9	0.28	<1	Tetrahydrofuran	42(100) 41(50) 72(30) 71(30) 43(20)
10	0.29	<1	Methylcyclopentane	56(100) 41(40) 69(40) 55(30) 42(20)
11	0.30	1-10	1,1,1-Trichloroethane	97(100) 96(65) 61(55) 31(20) 117(103) 119(113) 21(5)
12	0.32	<1	Benzene	78(100) 77, 90-92(20)
13	0.57	<1	Toluene	91(100) 92(60)
14	0.91	<1	C ₇ Alkyl Benzene	91(100) 106(40)
15	0.97	<1	C ₈ Alkyl Benzene	91(100) 106(45)
16	1.00	-(8)	1,5.	75(100) 77(33) 110(30) 61(25)
17	1.00	<1	Methylethyl Cyclohexane	55(100) 97(55) 41(30) 126(8)
18	1.01	<1	Methylethyl Cyclohexane	55(100) 97(80) 41(20) 126(15)
19	1.05	<1	Methylethyl Cyclohexane	55(100) 97(95) 41(55) 126(12)
20	1.06	<1	Methylethyl Cyclohexane	55(100) 97(90) 96(40) 81(40) 126(18)
21	1.09	<1	C ₈ Cyclohexane	55(100) 82(80) 81(70) 41(50) 67(45) 126(10)
22	1.10	<1	Methylethyl Cyclohexane	97(100) 55(98) 41(30) 69(25) 126(8)
23	1.11	<1	C ₈ Cyclohexane	81(100) 55(98) 82(16) 51(40)
24	1.14	<1	Diethyl Cyclohexane	69(100) 111(70) 55(50) 41(38)
25	1.15	<1	M 126 Hydrocarbon	57(100) 71(70) 43(65)
26	1.17	<1	4-n-Propylheptane	57(100) 43(48) 98(35)
27	1.18	<1	Unknown Hydrocarbon	69(100) 70(70) 55(65) 125(60)

TABLE A-2. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 1E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum	Mass Spectral Reference Match Compound	R.I. ± 10
1	929	aa	Branched Hydrocarbon C > 9	43 (100) 57 (88) 41 (76) 85 (34) 71 (25) 56 (25) 118 (3)	Nonane	546
2	1010	aa	Branched Hydrocarbon C > 10	43 (100) 57 (90) 41 (70) 71 (35) 85 (25) 162 (3)	Decane	576
3	1102	aa	Unknown		Undecane	583
4	1202	a	Silicone	267 (100) 73 (30) 268 (25) 251 (16) 269 (16)		
5	1211	a	Branched Hydrocarbon C > 12	43 (100) 57 (99) 41 (79) 71 (32) 85 (32) 170 (3)	Undecane	530
6	1685	aa	Hexamethylbenzene	Internal Standard		
7	1704	a	Heptadecane		Heptadecane	577
8	1716	a	Branched Hydrocarbon C > 17		Heptadecane	583
9	1834	a	Methylphenanthrene	192 (100) 191 (62) 189 (31) 193 (22) 165 (18)	2-Methylphenanthrene	583
10	1884	a	?		2-Methylphenanthrene	578
11	1905	a	Phthalate		1,2-benzenedicarboxylic Acid butyl, 2-Methylpropyl Ester	676
12	1978	a	C ₂ -Phenanthrene	206 (100) 191 (33) 189 (29) 205 (23) 207 (20)	1,4-Dimethylphenanthrene	679
13	1994	a	C ₂ -Phenanthrene		2,3-Dimethylphenanthrene	520
14	2109	a	C ₃ -Phenanthrene + Alkane	205 (100) 57 (93) 43 (86) 71 (60) 220 (56) 85 (62)		
15	2129	a	C ₃ -Phenanthrene		2,3,5-Trimethylphenanthrene	638
16	2135	a	C ₃ -Phenanthrene		2,3,5-Trimethylphenanthrene	671
17	2184	aa	Pentadecylbenzene	Internal Standard		
18	2204	a	?			
19	2215	a	Phosphate, Trifluoride	57 (100) 70 (98) 41 (68) 55 (66) 100 (50) 83 (60) 112 (38)	Phosphoric Acid, Triisopropyl Ester	563
20	2295	a	?	57 (100)	Decane 1,6-Bis(2,2-Dimethyl-Propylidene)	520
21	2347	a	Branched Hydrocarbon C > 23	57 (100) 71 (80) 85 (60) 43 (60)	Decane	608
22	2394	a	Branched Hydrocarbon C > 23	57 (100)	Decane, 11-Nonyl-	633
			Gas chromatogram looks like a typical gasoline hydrocarbon mixture.			

TABLE A-3. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 1E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification Before Methylation	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Name	R.I. $\mu\text{g/l}$
1	1022	*	Branched Fatty acid C ≥ 7	87 (100) 102 (65) 57 (43) 55 (33) 41 (30)	Heptanoic Acid, 2-Ethyl H.E.	660
2	1034	*	1	89 (100) 125 (96) 53 (75) 127 (61) 63 (48) 126 (30)		
3	1140	*	1	133 (100)		223
4	1329	*	7	Poor Mass Spectrum		
5	1685	ss	Hexaethylbenzene	Internal Standard		
6	1704	*	Tetradecanoic Acid	76 (100) 87 (50)	Tetradecanoic Acid H.E.	438
7	1887	*	7	41 (100)	10-Undecanoic Acid H.E.	386
8	1913	*	Fatty Acid C ≥ 10	76 (100) 87 (55)	Pentadecanoic Acid H.E.	630
9	1983	*	Phthalate	149 (100) 41 (18) 71 (6) 150 (10)	1,2-Benzenedicarboxylic Acid butyl, 2-methylpropyl Ester	469
10	2073	*	Fatty Acid C ≥ 17	67 (100)	9,12-Octadecadienoic Acid H.E.	220
11	2083	*	Fatty acid C ≥ 17	41 (100)	10-Undecanoic Acid H.E.	465
12	2089	*	Fatty Acid C ≥ 17	55 (100) 69 (69) 79 (43) 87 (33) 41 (60) 43 (48)	11-Octadecenoic Acid H.E.	287
13	2112	ss	Fatty Acid C ≥ 18	76 (100)	Tetradecanoic Acid H.E.	632
14	2185	ss	Pentadecylbenzene	Internal Standard		
15	2209	*	7	117 (100)	3-Ictanoic Acid, 4-Phenyl-butyl Ester	148

TABLE A-4. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 1E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Name	R.I. $\mu\text{g/l}$
5	1669	ss	Hexaethylbenzene	Internal Standard		
10	1921	*	Phthalate	149 (100)	1,2-Benzenedicarboxylic Acid butyl, 2-methylpropyl Ester	473
11	2183	ss	Pentadecylbenzene	Internal Standard		

TABLE A-5. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 2VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	--	Air	44(100)
2	0.14	1-10	Bucene	41(100) 56(50)
3	0.16	1-10	Trichlorofluoromethane	101(100) 103(66)
4	0.17	1-10	Dichloroethylene	81(100) 98(80) 98(55)
5	0.17	1-10	Dichloromethane	49(100) 51(33) 84(85) 86(55)
6	0.17	1-10	Carbon Disulfide	78(100) 80(5) 94()
7	0.20	1-10	2,3-Dimethylbutane	43(100) 42(55) 41(39) 71(30) 57(18)
8	0.20	<1	Butyraldehyde	44(100) 72(40) 41(25) 57(15)
9	0.21	1-10	Methyl ethyl Ketone	43(100) 72(20) 57(10) 78(7) ?
10	0.21	1-10	3-methylpentane	57(100) 58(9) 51(95) 53(8) 86(3)
11	0.23	1-10	Hexane	57(100) 41(100) 43(80) 56(60) 86(12)
12	0.26	1-10	Methyl Cyclopentane	56(100) 41(65) 89(40) 86(8)
13	0.27	1-10	1,1,1-Trichloroethane	97(100) 99(70) 41(60) 63(48) 117(10) 119(8)
14	0.29	<1	Benzene	78(100) 51-53(20)
15	0.30	<1	Carbon Tetrachloride	119(100) 117(90) 71(60) 82(50) 86(40) 121(35)
16	0.31	<1	Cyclohexane	58(100) 41(60) 86(80) 55(55) 42(40)
17	0.37	<1	Trichloroethylene	95(100) 60(85) 40(70) 97(60) 130(40) 132(40) 134(40) [Weak]
18	0.55	1-10	Toluene	91(100) 92(60)
19	0.88	<1	C ₇ Alkyl Benzene	91(100) 106(30) 92(10)
20	0.91	<1	C ₇ Alkyl Benzene	91(100) 106(40) 105(20) 92(10)
21	0.96	<1	Styrene	104(100) 78(90) 103(70) 51(55) 77(30)
22	0.98	<1	C ₇ Alkyl Benzene	91(100) 106(40) 103(20)
23	1.00	-(8)	1,5, (Trichloropropane)	75(100) 77(33) 81(28)
24	1.06	<1	Alkane	43(100) 57(90) 41(55) 85(40) 99(16)
25	1.23	<1	Alkane	57(100) 41(30) 43(30) 71(28) 85(10)
26	1.24	1-10	C ₈ H ₁₈ Hydrocarbon e.g. 1-methyl Cyclohexene	94(100) 79(63) 80(60) 107(50) 108(40) 92(30)
27	1.31	<1	Alkane	57(100) 41(90) 71(50) 85(40)
28	1.51	<1	Alkane + C ₇ Alkyl Benzene	97(100) 41(73) 71(50) 41(55) 85(28) 119(20) 121(34) 103

TABLE A-6. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 2E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification before Methylation	Characteristic Ions in Mass Spectrum		Mass Fragmentation Scheme (m/z)	
	1683	..	Nonethylbenzene	Internal Standard			
1	1710	a	Tetradecanoic Acid	76 (100) 87 (73) 41 (56) 55 (36) 143 (12) 211 (5)			313
2	1911	a	Hexadecanoic Acid	76 (100) 87 (60)			516
3	1921	a	Phthalate, Dibutyl	149 (100)			319
4	1982	a	?	Weak Spectra			
5	2071	a	Alkanoic acid C $\geq$ 18	67 (100)			423
6	2082	a	Alkanoic Acid C $\geq$ 18	55 (100)			642
7	2111	a	?	171 (100) 191 (100) 91 (91) 221 (87) 89 (83) (Mixture)			209
8	2121	a	Branchal alkane acid C $\geq$ 18	76 (100) 87 (70) 55 (35) 148 (16) 179 (5)			403
9	..	..					
10	2139	a	Subst. Cyclohexane Acid	146 (100) 101 (60) 136 (63) 91 (57) 41 (46) 92 (52) 187 (48)			210
11	2158	a	Subst. Cyclohexane Acid	146 (100) Weak Spectra			
12	2170	..	Pentadecylbenzene	Internal Standard			317
13	2181	..	Subst. Phenanthrene Acid	59 (100) 41 (83) 91 (71) 67 (70) 241 (56) 242 (44) 302 (18) 121 (106)			363
14	2197	a	Subst. Phenanthrene Acid	121 (100) 91 (33) 55 (29) 59 (28)			369
15	2210	a	Subst. Phenanthrene Acid	121 (100)			369
16	2228	a	Subst. Phenanthrene Acid	41 (100) Weak Spectra			200
17	2267	a	Subst. Phenanthrene Acid	41 (100) 81 (92) 91 (90) 105 (90) 79 (88) 241 (56) 242 (33)			312
18	2304	..	Subst. Phenanthrene Acid	239 (100) 59 (78) 63 (67) 41 (63) 260 (58)			387
19	2360	..	Subst. Phenanthrene Acid	41 (100)			287
20	2527	a	Subst. Phenanthrene Acid	59 (100) 233 (85) 254 (78) 187 (69) 211 (66) 213 (66) 329 (18)			218

TABLE A-7. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 3VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	--	Air	44(100)40(2)
2	0.12	--	Dimethylether	45(100)46(45)
3	--	--	Air	44(100)40(5)
4	0.13	10-100	Dimethylether	45(100)46(60)
5	0.17	10-100	Dichloroethylene	96(100)61(95)98(70)83(60)
6	0.17	10-100	Dichloromethane	69(100)84(80)86(55)51(25)
7	0.20	1-10	2,3-Dimethylbutane	63(100)42(45)71(30)41(15)
8	0.21	1-10	Methylethyl ketone	63(100)72(30)
9	0.23	10-100	Hexane	57(100)43(60)56(45)41(40)83,85,80(12)
10	0.26	1-10	Methyl cyclopentane	56(100)69(60)41(35)84(10)
11	0.27	10-100	1,1,1-Trichloroethane	97(100)99(66)61(40)63(20),117(10)
12	0.37	1-10	Trichloroethylene	95(100)97(70)130(90)132(85)
13	0.55	1-10	Toluene	91(100)92(60)
14	1.00	-(8)	1.S.	75(100)110(60)112(45)
15	1.02	1-10	Alkane	57(100)56(45)71(20)85(18)
16	1.06	<1	Alkane	71(100)43(60)57(50)113(22)
17	1.11	<1	Alkane	57(100)43(50)41(30)70(22)71(20)98(15)
18	1.23	1-10	Alkane	57(100)71(25)85(20)
19	1.25	<1	Alkane	57(100)56(55)41(32)71(18)85(20)99(10)

TABLE A-8. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 4VI-a

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.13	1-10	Dimethylbutane	41(100)56(62)39(58)
3	.14	1-10	Chloroethane	64(100)66(35)49(15)
4	.15	1-10	Acetone + Dimethyl ether (T)	45(100)43(65)46(35)58(20)
5	.16	<1	Unknown (very weak)	59(100)110(96)108(96)74(60)
6	.16	20-30	Dichloromethane	49(100)84(67)
7	.17	1-10	Methylethyl ketone	43(100)41(83)72(90)
8	.18	1-10	Crotonaldehyde	41(100)39(85)70(92)
9	.22	1-10	Chloroform	83(100)85(66)
10	.22	1-10	Di-n-propoxy ethane	45(100)43(40)87(12)
11	.23	<1	Chlorobutene	55(100)90(50)92(12)
12	.23	1-10	Chlorobutene	55(100)39(50)90(35)92(10)
13	.24	1-10	Tetrahydrofuran	42(100)41(72)71(53)72(52)
14	.24	1-10	1,2-dichloroethane	62(100)49,64(32)98(10)100(8)
15	.32	10-20	Dichloropropane	63(100)62(70)41(35)76(32)
16	.38	1-10	C_7H_{16}	43(100)71(70)57(60)100(20)
17	.51	1-10	Toluene	91(100)92(62)
18	1.00	8	I.S.	75(100)110(33)
19	1.06	1-10	Diethyl disulfide	66(100)122(90)96(65)
20	1.14	1-10	1-Bromo-2,3-dichloro propane	111(100)75(75)113(65)77(25)124(10)

TABLE A-9. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 4VI-6

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.14	--	Air	44 (100)
2	.15	1-10	Chloromethane	50 (100) 44 (34) 57 (30)
3	.16	1-10	1,3-Butadiene	39 (100) 54 (60) 53 (65)
4	.17	1-10	Unknown	56 (100) 55 (72)
5	.17	10-100	Acetone	43 (100) 58 (25) 44 (25)
6	.18	≈ 10	Chloropropene	41 (100) 39 (85) 76 (30) 59 (20) 78 (8)
7	.19	≈ 10	Dichloromethane	84 (100) 49 (98)
8	.	1-10	Carbon Disulfide	76 (100) 44 (28) 78 (8)
9	.23	1-10 ea	Chloroform + Alkane	41 (100) 57 (96) 43 (80) 83 (78) 85 (50) 130 (12)
10	.	1-10	Tetrahydrofuran	42 (100) 72 (30) 71 (29)
11	.	1-10	Vinylchloride (?)	62 (100) 64 (33) 35 (10)
12	.29	1-10	Benzene	78 (100)
13	.35	1-10	Trichloroethylene	95 (100) 44 (82) 130 (70) 132 (68) 97 (62)
14	.54	1-10	Toluene	91 (100) 92 (60)
15	.66	1	Tetrachloroethylene	166 (30) 129 (29) 131 (27) 164 (24)
16	.89	1	Ethyl benzene	91 (100) 106 (30)
17	.93	1	Xylene	91 (100) 106 (30)
18	1.00	(-) 8	I.S.	75 (100) 110 (30)

TABLE A-10. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 4VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12		Air	44(100)
2	0.19	10-100	Dichloromethane	49(100)84(62)86(40)
3	0.25	10-100	Chloroform	83(100)85(70)87(12)
4	0.28	<1	C_6H_{12} , e.g., Hexane or Methylcyclopentane	56(100)41(60)69(38)84(5)
5	0.29	<1	Trichloroethane	97(100)61(70)99(70)63(20)
6	0.31	<1	Benzene	78(100)
7	0.32	<1	Carbon tetrachloride	119(100)117(95)82(40)47(40)
8	0.38	1-10	Bromodichloromethane	83(100)85(60)47(25)127(8)129(10)131(5)
9	0.56	1-10	Toluene	91(100)92(60)
10	0.60	1-10	Dibromochloromethane	129(100)127(80)113(30)79,81(25)
11	0.88	1-10	C_2 Alkyl benzene	91(100)106(30)
12	0.89	<1	Bromoform	173(100)171(50)175(48)254(10)
13	0.91	1-10	C_2 Alkyl benzene	91(100)106(45)
14	0.98	1-10	C_2 Alkyl Benzene	91(100)106(40)
15	1.00	-(8)	I.S.	75(100)77(30)
16	1.07	<1	C_3 Alkyl benzene	105(100)120(30)
17	1.15	1-10	C_3 Alkyl benzene	91(100)120(25)
18	1.17	1-10	C_3 Alkyl benzene	105(100)120(30)
19		<1	C_3 Alkyl benzene	105(100)120(40)

TABLE A-11. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 41-a

GC Peak No.	Retention Index	Amount, µg/l	Terpene Identification	Characteristic ions in Mass Spectrum	Most Reasonable Monomer Match Compound	R.I. ± 10
1	852	a		43 (100) 78 (86) 91 (76) 43 (71) 92 (45) 117 (32) 89 (35) 131 (12)		
6	882	a	?	43 (100) 59 (54) 101 (43) 49 (34) Poor spectra		
7	896	a	?	43 (100) 59 (53) 101 (22) 51 (20) 78 (15) Poor Spectra		
10	958	a	?	85 (100) 43 (99) 58 (65) 59 (31) 115 (22) 131 (18)		
11	996	a	?	85 (100) 43 (99) 45 (78) 58 (41)		
13	1030	a	?	57 (100) 85 (88) 41 (42) 93 (36) 63 (32) 105 (26) Poor spectra		
14	1040	a	?	69 (100) 68 (49) 34 (35) 61 (32) 78 (18)		
15	1138	aa	Ethyl Benzenemethanol	107 (100) 78 (58) 77 (35) 105 (13) 136 (8) 51 (7)	Benzeneethanol, alpha-Ethyl-	625
16	1146	a	1-Phenyl-1-Propanone	105 (100) 77 (43) 134 (11) 51 (10)	1-Propanone, 1-Phenyl-	672
21	1340	a	?	71 (100) 43 (67) 60 (28) 81 (23) 56 (24) 55 (23) 89 (20) 98 (18) Poor spectrum	1-Heptanol, 5-Methyl-	257
22	1356	a	?	71 (100) 43 (70) 56 (64) 89 (59) 143 (12) 173 (11)	1-Heptanol, 4-(Benzylonyl)-	279
25	1921	a	Phthalate, Dibutyl	149 (100) 150 (9) 104 (8) 41 (7) 76 (5) 205 (2)	1,2-Hexanedicarboxylic acid, Butyl-2-Methyl Propyl Ester	495
26	2182	aa	Pentadecylbenzene	Internal standard		
*	1682	aa	Hexaethylbenzene	Internal standard		

TABLE A-12. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 41-b

GC Peak No.	Retention Index	Amount, µg/l	Terpene Identification	Characteristic ions in Mass Spectrum	Most Reasonable Monomer Match Compound	R.I. ± 10
1	983	aa	1,1'-Oxy Bis [2-Ethonyl-Ethene (Carbitol)]	45 (100) 59 (38) 72 (21) 43 (23) 104 (5)	Ethane 1,1'-Oxy Bis [2-Ethonyl]	611
4	1125	a	Acenaphthalene 1,2 Dithio	134 (100) 153 (35) 152 (25) 155 (12) 76 (13) 63 (7) 51 (8)	Acenaphthalene, 1,2-Dithio	408
5	1247	a	Benzenesulfonic Acid 4-Methyl Hydrazide	91 (100) 155 (43) 65 (33) 186 (20)	Benzenesulfonic acid 4-methyl hydrazide	194
8	1373	a	Benzenesulfonamide N,4-Methyl	91 (100) 155 (22) 65 (27) 151 (23) 185 (23)	Benzenesulfonamide N,4-Dimethyl	434
9	1445	a	Fatty Acid C ₁₆	76 (100) 87 (59) 43 (21) 51 (18) 143 (13)		
10	1678	a	Sub anthracene acid	253 (100) 91 (30) 254 (28) 77 (23) 195 (20)		
14	2087	a	Fatty Acid C ₁₇	55 (100) 74 (86) 87 (58) Poor MS		
15	2112	a	Octadecanoic Acid	76 (100) 87 (63) 64 (33) 143 (11) 199 (2)	Heptadecanoic Acid M.E.	522
16	2182	aa	Pentadecylbenzene	Internal standard		
*			Palmitic Acid	Internal standard		

TABLE A-13. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 41-b

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Boreman Match Compound	S.I. $\times 10^3$
1	873	a	?	83(100)42(50)41(47)56(43)69(27)97(17)	7-Oxabicyclo[4.1.0.]heptane	568
2	881	a	?	85(100)63(53)58(48)131(22)115(21)71(20)105(7)165(2)	Ethene, (2-Ethoxy-1-methoxyethoxy)-	252
3	956	a	?	85(100)57(80)61(32)58(22)93(14)142(13)127(6)	3-Pentanone, 2,2,4,4-Tetramethyl-	536
4	982	a	?	69(100)68(49)56(36)41(33)42(22)117(7)121(3)		
5	1076	a	2-bromocyclohexanol	81(100)57(61)99(28)79(18)132(4)178(2)180(1)	Cyclohexanol, 2-bromo-, C18-	664
6a	1135	aa	1-Phenyl-1-propan-1-one	105(100)77(52)51(18)134(10)		
6b	1135		2-Ethyl, Benzeneethanol	107(100)79(61)51(13)136(8)		
11	2180	aa	Pentadecylbenzene	Internal standard		
a	1682	aa	Hexaethylbenzene	Internal standard		

TABLE A-14. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 4E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Reason Match	
					Compound	R.I. ± 10°
1	857	na	Unresolved peak	41 (100) 83 (76) 42 (63) 49 (52) 70 (43) 97 (11) 98 (8)		
2	878	a	?	35 (100) 70 (92) 42 (78) 98 (43) 41 (48) 69 (40)		
3	886	na	Chlorocyclohexane	81 (100) 79 (75) 80 (43) 41 (32) 51 (31) 116 (10) 118 (6)		
4	1003	na	4-Chlorocyclohexanol	57 (100) 80 (77) 44 (77) 41 (70) 81 (48) 88 (33) 98 (23) 134 (8) 136 (3)		
5	1015	a	?	41 (100) 57 (91) 43 (71) 55 (58) 70 (32) 83 (27)		
6	1022	a	Alkyl-cyclohexane	57 (100) 41 (71) 43 (53) 58 (35) 70 (23) 83 (18) 112 (2)		
7	1037	na	Dichlorocyclohexane	81 (100) 80 (70) 41 (28) 132 (1)		
8	1077	na	2-Bromocyclohexanol	81 (100) 57 (85) 41 (42) 99 (27) 132 (3) 178 (1) 180 (1)		
9	1118	na	Bromo, chlorocyclohexane	79 (100) 81 (98) 55 (85) 41 (78) 51 (42) 117 (36) 119 (13)	Cyclohexane, 1-Bromo-2-Chloro	240
10	1135	a	1-Phenylpropan-1-one	105 (100) 77 (40) 51 (20) 134 (12)	1-Propenone, 1-Phenyl	647
11	1194	a	1,3-Dibromocyclohexane	81 (100) 41 (21) 79 (23) 161 (10) 163 (10)	Cyclohexane, 1,3-Dibromo	406
12	1243	a	Dibromocyclohexane	81 (100) 41 (24) 79 (23) 117 (12) 244 (3) 246 (1)	Cyclohexane, 1-Bromo-2-Chloro	338
13	1264	a	Dihydro indanone (1)	104 (100) 132 (93) 78 (59) 103 (53) 51 (39) 131 (27)	1-H-Inden-1-one, 2,3-Dihydro	417
14	1269	a	Mixture? Bromo?	97 (100) 41 (82) 79 (79) 57 (43) 69 (42) 132 (39) 134 (27) 198 (2)		
15	1288	a	Ethanone, 1-(2,4-dimethylphenyl)	133 (100) 105 (61) 77 (31) 148 (28) 79 (25)	Ethanone, 1-(2,4-dimethylphenyl)-	635
16	1315	a	?	117 (100) 146 (86) 118 (52) 115 (42) 91 (31) 43 (30)	1-H-Indene, 1-Ethyl-2,3-Dihydro	449
17	1333	na	1-(2H)-Naphthalenone, 3,4-Dihydro	118 (100) 90 (100) 146 (87) 89 (60) 63 (33) 51 (25)	1-(2H)-Naphthalenone, 3,4-Dihydro	613
18	1353	a	C ₂ -Alkylidihydroindene	117 (100) 146 (62) 118 (55) 115 (37) 91 (30) 63 (20)	1-H-Indene-1-Ethyl-2,3-Dihydro	480
19	1387	a	C ₂ -Alkylidihydroindene	117 (100) 146 (75) 118 (50) 115 (37) 91 (34) 63 (32) 147 (18)	?	479
20	1369	a	Alkyl naphthalene	118 (100) 90 (95) 147 (88) 140 (60) 145 (55) 103 (50) 77 (38)	1-(2H)-Naphthalenone-3,4-Dihydro-2-Methyl	233
21	1441	a	?	104 (100) 77 (84) 132 (59) 51 (59) 160 (55) 41 (58) 213 (48) 211 (47) 244 (3)		
22	1458	a	?	165 (100) 57 (92) 41 (60) 180 (52) 137 (51) 234 (9) 236 (5)		
23	1467	a	?	117 (100) 115 (78) 213 (67) 211 (66) 226 (22) 228 (21)		
24	1508	a	?	118 (100) 117 (95) 115 (92) 90 (58) 180 (53) 246 (2) 248 (3)		
25	1520	a	?	196 (100) 125 (54) 198 (62) 160 (36) 276 (5) 278 (10) 280 (4)		
26	1557	a	?	115 (100) 117 (98) 224 (68) 226 (66) 196 (19) 198 (17)		
27	1591	a	?	118 (100) 90 (58) 115 (52) 144 (40) 224 (8) 228 (7)		
28	1602	a	?	115 (100) 117 (91) 63 (43) 226 (39) 224 (38) 282 (9) 294 (5)		
29	1628	a	?	117 (100) 242 (96) 126 (88) 161 (61) 240 (72) 224 (50) 226 (49)		
30	1650	a	?	115 (100) 117 (92) 224 (67) 226 (68) 128 (75) 91 (56) 290 (3) 293 (4)		

TABLE A-14. (Continued)

GC Peak No.	Retention Time, min	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Structural Match	K _L × 10 ³
31	1682	..	Hexamethylbenzene	Internal Standard		
32	1703	..	Mixture HC C & 17	211(100)213(99)57(100)115(85)117(83)292(85)290(42)299(37)		
33	1713	..	?	211(100)213(95)115(90)117(81)292(65)290(40)294(35)91(63)		
34	1899	..	Nonadecane	43(100)57(98)71(63)41(58)85(43)	Heptadecane, 2-Methyl	626
35	1921	..	Phthalate, Dibutyl	149(100)101(31)85(25)103(31)		
36	1958	..	Melo althane +?	85(100)101(43)135(38)87(31)107(28)115(30)	Cl ₁₈ -Pentane	358
37	2000	..	Elonsum +?	43(100)57(93)71(61)85(61)41(48)	Pentacosane	523
38	2101	..	Heptacosane	57(100)43(77)71(62)85(41)55(37)41(33)	Heptadecane, 9-Methyl	568
39	2141	..	Branched Hydrocarbon, C ≥ 21	57(100)43(66)71(58)85(33)55(33)	Elonsum-7-Methyl	551
40	2155	..	?	Peak unresolved on GC-MS		
41	2166	..	?	"		
42	2183	..	Pentadecylbenzene	Internal Standard		
..		..	High boiling Hydrocarbons			
..		..	Quantification data unreliable because of increased baseline in GC			

TABLE A-14. (Continued)

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Element Match	
					Compound	E.I. n 103
31	1682	ss	Hexaethylbenzene	Internal Standard		
32	1703	v	Mixture HC C & 17	211(100)213(99)57(100)115(85)117(83)282(85)290(42)298(37)		
33	1713	v	?	211(100)213(95)115(90)117(81)292(65)290(40)294(35)31(63)		
34	1899	v	Nonadecane	43(100)57(98)71(63)41(58)85(43)	Heptadecane, 2-Methyl	626
35	1921	v	Phthalate, Dibutyl	149(100)101(31)85(25)103(31)		
36	1958	v	Diethyl alkane +?	85(100)101(43)135(38)87(31)103(28)131(20)	C ₁₈ -F ₆ -Pentane	358
37	2000	v	Elcosane +?	43(100)57(93)71(61)85(61)41(48)	Pentacosane	523
38	2101	v	Heptacosane	57(100)43(77)71(62)85(41)55(37)41(33)	Heptadecane, 9-Methyl	548
39	2141	v	Branched Hydrocarbon C ≥ 21	57(100)43(66)71(58)85(33)55(33)	Elcosane-7-Methyl	551
40	2155	v	?	Peak unresolved on GC-MS		
41	2166	v	?	"		
42	2183	ss	Pentadecylbenzene	Internal Standard		
*		ss	High boiling Hydrocarbons			
		ss	Quantification data unreliable because of increased baseline in GC			

TABLE A-15. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 5VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Retention Identification	Characteristic ions in Mass Spectrum
1	0.13	--	Air	44(100)
2	0.17	<1	Butene	41(100) 56(40)
3	0.19	10-100	Acetone	43(100) 58(33)
4	0.20	1-10	Dichloromethane	49(100) 84(60)
5	0.24	<1	2,2-Dimethylbutane	43(100) 42(60) 71(10)
6	0.25	<1	3-Methylpentane (T)	57(100) 56(90) 41(80)
7	0.26	1-10	Heptane (T)	57(100) 41(80) 83(60) 56(50)
8	0.29	1-10	Methyl cyclopentane	56(100) 41(50) 69(40) 84(6)
9	0.57	1-10	Toluene	91(100) 92(50)
10	1.00	-(8)	1,5.	75(100)
11	1.19	<1	C ₇ Alkyl benzene	105(100) 120(45)
12	1.20	1-10	C ₇ Alkyl benzene	105(100) 120(40)
13	1.22	1-10	Alkane	57(100) 71(30) 85(15)
14	1.24	1-10	C ₇ Alkyl benzene	105(100) 120(45)
15	1.30	1-10	C ₇ Alkyl benzene	105(100) 120(40)
16	1.32	1-10	Propenyl benzene	117(100) 118(50) 115(40)
17	1.36	1-10	C ₈ Alkyl benzene	105(100) 119(95) 134(50) 91(32)
18	1.36	1-10	C ₈ Alkyl benzene	105(100) 134(25)
19	1.37	1-10	C ₈ Alkyl benzene	105(100) 91(30) 119(30) 134(30)
20	1.38	1-10	C ₈ Alkyl benzene	119(100) 134(30)
21	1.39	1-10	C ₈ Alkyl benzene	105(100) 134(20)
22	1.39	1-10	C ₈ Alkyl benzene	119(100) 134(30)
23	1.42	1-10	C ₈ Alkyl benzene	119(100) 134(20)
24	1.43	1-10	C ₈ Alkyl benzene	119(100) 134(20)
25	1.44	1-10	C ₈ Alkyl benzene	119(100) 134(20)
26	1.46	1-10	C ₈ Alkyl benzene	119(100) 134(20)
27	1.49	1-10	C ₈ Alkyl benzene	119(100) 134(20)
28	1.49	10-100	C ₈ Alkyl benzene	119(100) 134(20)
29	1.52	1-10	C ₁₀ H ₁₂ , n.p., (2-Methylpropyl) benzene	117(100) 132(40)

TABLE A-15. (Continued)

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
31	1.53	1-10	C ₁₀ H ₁₂	117(100)132(40)
32	1.54	1-10	C ₅ -Alkyl benzene	119(100)91(30)148(10)
33	1.54	1-10	C ₅ -Alkyl benzene	119(100)138(40)
34	1.55	1-10	C ₁₀ H ₁₂ (1,2,3,4-Tetrahydro naphthalene)	104(100)91(40)132(40)
35	1.57	1-10	C ₅ -Alkyl benzene	119(100)133(50)148(30)
36	1.58	1-10	Naphthalene	128(100)127(15)
37	1.59	1-10	C ₅ -Alkyl benzene	119(100)148(20)
38	1.63	1-10	C ₅ -Alkyl benzene	133(100)148(30)
39	1.64	1-10	C ₅ -Alkyl benzene	133(100)148(20)

TABLE A-16. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 5E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum	Ident. Retention Index Blank Compound	E.I. $\times 10^3$
2	887	a	?	42 (100) 41 (40) 70 (32) 86 (28) 97 (18) 98 (15) Poor mass spectra		
3	899	a	Nonane			
6	1002	a	Decane			
10		a				
13	1073	a	2-Bromocyclohexanol	81 (100) 37 (32) 99 (26) 136 (5) 137 (6) 180 (2) 178 (1)	Cyclohexanol, 2-bromo	432
14	1085	a	?	Poor spectra	Benzenes, 2-ethyl, 2,4-dimethyl	244
15	1098	a	Hydrocarbon Undecane			
16	1101	a	C ₄ Alkylbenzene	119 (100) 136 (37) 91 (23) 207 (5)	Benzenes, tetramethyl	376
17	1111	a	1-Bromo-2-Chlorocyclohexane	81 (100) 79 (22) 117 (12) 33 (10) 196 (3) 198 (2) 100 (1)	Cyclohexanes, 1-bromo-2-chloro	525
18	1116	a	C ₅ -Alkylbenzene	107 (100) 105 (49) 132 (40) 148 (20) 105 (19)	Benzenes (2-methyl-1-propenyl)	393
19		a	?	104 (100) 132 (38) 91 (29) 78 (22)	18-Indene-1,2-diol, 2,3-dihydro	423
20		a	Naphthalene	128 (100) 102 (11) 51 (8)	Anulene	326
21		a	C ₅ -Alkylbenzene	132 (100) 136 (45) 91 (43) 148 (40) 105 (32) 104 (24) Poor spectra	Benzenes, pentamethyl-	255
22	1210	a	Dibromocyclohexane	81 (100) 127 (51) 79 (30) 112 (29) 244 (5)	Cyclohexanes, 1,3-dibromo-	169
23	1289	a	?	132 (100) 117 (87) 115 (45) 91 (41) 146 (29) 150 (23) 216 (6) 212 (5)		
24	1323	a	C ₂ -Alkylidihydronaphthalene	130 (100) 120 (83) 119 (82) 147 (54) 91 (52) 148 (42)		
26	1354	a	1 (28)-Naphthalenone, 3,4-dihydro	118 (100) 146 (63) 90 (48) 89 (26)	Ethanone, 1-(2,4,6-trimethylphenyl)-	344
27	1440	a	?	107 (100) 125 (67) 79 (42) 77 (41) 136 (37) 152 (26)	1 (20)-Naphthalenone, 3,4-dihydro-	450
28	1628	a	Tributyl Phosphate	99 (100) 155 (23) 125 (10) 211 (8) 41 (9) 37 (6)	Phosphoric acid tributyl ester	591

TABLE A-17. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 6VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12		Air	44(100)
2	0.18	10-100	Dichloromethane	49(100)84(80)
3	0.22	<1	2,3-Dimethylbutane	43(100)42(50)41(40)71(20)
4	0.23	<1	3-Methylpentane	57(100)56(90)41(90)
5	0.24	1-10	Chloroform + C_6 Alkane	41(100)27(95)43(12)83(60)
6	0.25	1-10	Isopropyl ether	45(100)43(28)87(27)102(2)
7	0.27	1-10	1,2-Dichloroethane	62(100)64(33)49(25)98(8)100(6)
8	0.36	1-10	1,2-Dichloropropane	63(100)41(75)62(70)76(50)97(5)112(3)
9	0.56	1-10	Toluene	91(100)92(60)
10	1.00	(8)	I.S.	75(100)77(33)

TABLE A-18. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 6E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Match	LI # 192
1	881	a	3-Heptanone	57(100)41(35)85(20)72(15)43(15)114(6)	3-Heptanone	676
2	895	a	?	85(100)43(98)45(90)58(63)71(26)115(15)131(15)	2-Pentanone, 3-methyl	321
3	915	a	?	45(100)43(83)85(68)42(48)57(35)81(25)	"	480
4	937	a	?	57(100)85(78)41(32)93(48)142(12)	3-Pentanone, 2,2,4,4-Tetramethyl	263
5	983	a	?	68(100)41(76)88(50)42(46)54(61)121(3)	Propenenitrile, 2-methyl	504
6	1040	a	Acetophenone	105(100)77(90)51(42)120(23)43(20)50(20)	Ethylene, 1-Phenyl	706
7	1095	a	Isophorone	82(100)138(16)54(18)41(16)	2-Cyclohexen-1-one, 3,3,5-Trimethyl	547
8a	1137	aaa	1-Phenyl-1-Propanone	105(100)77(80)51(43)59(21)134(10)	Benzocyclohexanone, Ethyl	485
8b	1137		4a-Ethyl Benzocyclohexanone	107(100)79(88)77(52)51(15)136(10)		
9	1131	a	?	81(100)105(83)77(52)41(48)99(30)148(6)		
10	1158	a	?	41(100)55(83)99(62)116(43)69(42)	2-Propanoic Acid, 2-methyl Pentyl Ester	358
11	1225	a	HC + ?	70(100)41(80)55(71)42(43)69(39)112(16)	2-Octene	738
12	1340	a	?	43(100)71(83)41(40)81(25)		
13	1355	a	?	43(100)71(86)36(70)89(38)41(50)143(5)173(5)	Butane, 2,2'-[Methylenebis(methyl)] 353	
14	1432	a	?	73(100)41(60)55(50)88(47)101(38)119(17)176(5)	1-Butanol, 4-(Nonyloxy)	522
15	1681	aa	Hexamethylbenzene	Internal Standard		
16	1920	a	Phthalate, Dibutyl	149(100)41(20)76(10)205(3)	1,2-Benzene dicarboxylic acid, butyl-2-methylhexyl ester	532
17	2181	aa	Pentadecylbenzene	Internal standard		
18	2458	a	Alkyl Benzene	91(100)113(18)57(17)71(12)		
19	2512	a	Phthalate, Bis(2-methylhexyl)	149(100)57(43)71(30)167(28)	1,2-Benzene dicarboxylic acid-Bis(2-methylhexyl) ester	363
20	2744	a	?	59(100)55(73)72(73)43(60)41(60)281(2)	9-Octadecanamide	501
21	2807	a	Alkylpyrene	69(100)81(55)41(42)95(15)	Tetradecanone-Hexamethyl-	516

TABLE A-19. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 7VI

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12		Air	44(100)
2	0.18	10-100	Dichloromethane	49(100)84(50)
3	0.21	1-10	2,3-Dimethylbutane	43(100)42(55)41(50)71(30)
4	0.22	1-10	3-Methylpentane	57(100)41(90)56(88)71(6)86(4)
5	0.24	1-10	C ₆ Alkane + Chloroform	57(100)41(95)43(70)56(55)83(30)
7				44(100)45(90)41(40)43(32)
8	0.27	1-10	Methyl cyclopentane	56(100)41(55)69(40)84(6)
9	0.28	1-10	Trichloroethane	97(100)99(70)61(50)119(10)117(8)
11	0.56	1-10	Toluene	91(100)92(60)
12	1.00		I.S.	75(100)110(50)77(33)
13	1.26	10-100	Dichlorobenzene	146(100)148(70)111(33)113(12)
14	1.27	10-100	Dichlorobenzene	146(100)148(70)111(35)113(10)

TABLE A-20. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 7VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	--	--	Air	44(100)
2		10-100	n-Pentane	43(100)42(95)41(90)57(22)72(12)
3		1-10	Dichloroethylene	61(100)96(60)98(40)63(35)100(4)
4		1-10	Dichloroethane	49(100)84(98) Set'd
5		<1	2,3-Dimethylbutane	43(100)42(58)41(48)71(20)
6		<1	3-Methylpentane	41(100)57(90)56(80)43(28)71(4)86(2)
7		<1	Chloroform	83(100)85(62)57(40)
8		1-10	Isopropyl ether	45(100)43(33)87(25)102(2)
9		1-10	Methyl cyclopentane	56(100)41(62)69(40)84(8)
10		1-10	Trichloroethane	97(100)99(62)61(55)117,119,121
11		1-10	Carbon tetrachloride	119(100)117(95)121(40)82(40)
12		1-10	Toluene	91(100)92(55)
13		1-10	n-Butyl ether	57(100)41(31)87(25)130(2)
14		10-100	Dichlorobenzene	146(100)148(70)111(45)113(15)
15		10-100	Dichlorobenzene	146(100)148(65)111(50)113(18)

TABLE A-21. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 71

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Name Match Compound	R.I. ± 10
5	985	a	1,3-Dichlorobenzene	146 (100) 148 (61) 111 (48) 75 (22) 50 (13) 113 (13) 150 (10)	Benzene, 1,3-Dichloro-	588
6	991	a	1,4-Dichlorobenzene	146 (100) 148 (63) 111 (37) 75 (30) 50 (18) 113 (18) 150 (11)	Benzene, 1,4-Dichloro-	566
8	1014	aa	1,2-Dichlorobenzene	146 (100) 148 (65) 111 (43) 75 (28) 50 (15) 113 (11) 150 (11)	Benzene, 1,2-Dichloro-	632
9	1098	a	Trichlorone	82 (100) 138 (22) 54 (16) 92 (11) 67 (9)	2-Cyclohexan-1-one, 3,5,5-Trimethyl	289
10	1100	a	Undecane	57 (100) 43 (46) 71 (50)	Decane, 2,2-Dimethyl-	564
11	1136	a	1,2,3,4-Tetrahydronaphthalene	104 (100) 132 (39) 91 (30) 113 (18) 117 (13) 78 (12)	Naphthalene, 1,2,3,4-Tetrahydro-	512
12	1156	a	Naphthalene	128 (100) 127 (21) 102 (15) 129 (13)	Naphthalene	540
13	1300	a	Tridecane			
14	1325	a	C ₇ -Alkyldihydronaphthalene	130 (100) 115 (75) 120 (74) 129 (65) 91 (40) 105 (33) 128 (39)	Benzene, 1,4-Dimethyl-2-(2-Methyl Propyl)	268
15	1331	aa	1(2H)-Naphthalene, 3,4-Dihydro	118 (100) 146 (59) 90 (51) 89 (23) 63 (11) 147 (6)	1(2H)-Naphthalene, 3,4-Dihydro-	662
16	1367	a	1,1'-Biphenyl	154 (100) 153 (40) 152 (31)	1,1'-Biphenyl	716
17	1368	a	Diphenyl Ether	170 (100) 161 (65) 142 (42) 77 (41) 51 (30) 169 (29) 115 (27) 171 (15)	Benzene, 1,1'-Diphenyl-	502
18	1682	aa	Hexaethylbenzene	Internal standard		
19	2182	aa	Pentadecylbenzene	Internal standard		
20	2810	a	Phthalene			
a	1129	a	1-Phenyl, 1-Propanone			

TABLE A-22. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 7E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Typical Identification	Characteristic ions in Mass Spectrum	Most Reasonable Chemical Structure	Ref. No.
1	887	5	n-Butyl Ether	57(100)41(39)87(13)56(20)101(6)	Benzene, 1,1'-Dyble	543
2	905	5	2-Butoxyethanol	57(100)41(73)43(40)87(23)43(18)75(10)	Ethanol, 2-Butoxy	877
3	985	5	1,3-Dichlorobenzene	146(100)148(65)111(43)75(43)74(32)50(35)150(10)	Benzene, 1,4-Dichloro	509
4	990	5	1,4-Dichlorobenzene	146(100)148(63)111(43)75(41)50(28)150(10)	Benzene, 1,2-Dichloro	492
5	1003	5	?	57(100)43(46)41(67)124(23)62(38)71(30)25(20)	Benzene, 1,2-Dichloro	429
6	1014	5	1,2-Dichlorobenzene	146(100)148(63)111(43)75(55)50(42)150(10)	2-Cyclohexan-1-one, 3,5,5-Trimethyl	423
7	1094	5	Tetraphenol	82(100)36(21)136(17)41(17)	Asiaron	558
8	1100	5	Undecane	43(100)37(40)41(48)71(40)85(23)	3-Pentadecane, 2,4,4-Tetramethyl	403
9	1136	5	1,2,3,4-Tetrahydronaphthalene	104(100)91(47)132(40)78(25)31(20)	2-Pentadecane, 4-Methyl-4-Phenyl	612
10	1136	5	Naphthalene	126(100)127(13)129(11)102(13)51(13)	1-(20)Naphthalene, 3,4-Dihydro	551
11	1193	5	Alkyl-diketone, n-alkyl	57(100)41(93)43(82)58(58)85(55)109(26)127(22)	Benzene, 1,1'-Dyble	562
12	1269	5	2-Pentadecane, 4-Methyl-4-Phenyl	161(100)91(72)119(48)176(41)41(42)43(42)	Phenol, 2,4-Bis(1-Methylbutyl)-	582
13	1331	5	1,2,3,4-Tetrahydronaphthalene-1-one	118(100)90(92)146(43)89(43)33(29)	Ethanol, 2-[2-(2-Butoxyethoxy)ethoxy]-	658
14	1359	5	?	Poor mass spectra (too weak)	Phenol, 2,4-Bis(1-Methylbutyl)-	251
15	1348	5	Diphenyl Ether	170(100)51(70)77(66)141(62)142(41)115(26)	Phenol, 2,4-Bis(1,1-Dimethylbutyl)-4-methyl	218
16	1397	5	Phenol, 2,4-Bis(1-Methylbutyl)-	165(100)121(27)178(23)107(19)91(21)	Phenol, 2,4-Bis(1-Methylbutyl)-	330
17	1420	5	Ethanol, 2-[2-(2-Butoxyethoxy)-	57(100)41(73)43(53)75(28)85(23)	Phosphoric Acid Triethyl Ester	499
18	1438	5	Subst. Phenol	165(100)178(30)135(35)	Naphthalene, 1,2,3-Trimethyl-4-Propenyl	236
19	1506	5	2,4-Bis(1,1-Dimethylbutyl)-4-methyl phenol	205(100)43(81)41(65)91(32)220(21)177(18)	Internal standard	
20	1554	5	Alkyl Benzene	43(100)41(76)91(40)	1,2-Nominalcarboxylic acid-Bis-2-Phenyl	532
21	1566	5	Isomer of #19	205(100)43(83)41(50)220(21)	Phenol, 2,4-Bis(1-Methylbutyl)-	187
22	1630	5	Triethyl Phosphate	99(100)41(28)135(12)211(5)	Phenol, 2,4-Bis(1-Methylbutyl)-	
23	1657	5	?	195(100)165(23)146(16)210(8)	Phenol, 2,4-Bis(1-Methylbutyl)-	
24	1682	5	Benzothienone	Internal standard		
25	1690	5	Phthalate	61(100)149(40)71(23)104(10)189(8)		
26	1707	5	?	63(100)205, 220 Poor spectra		
27	1759	5	?	189(100) Poor spectra		
28	1863	5	?	175(100)94(35)174(30)286(5) Poor spectra		
29	1880	5	?	220(100)227(83)115(92)77(18)		
30	1887	5	Phthalate	146(100)147(35)140(10)105(43)77(13)		

TABLE A-22. (Continued)

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Pronounced Element Molar Ratios	
					Compound	R, I n, 10 ³
31	1941	a	1,1'-Biphenyl, 2-Phenoxy	77(100)246(79)152(60)115(60)51(53)245(18)	1,1'-Biphenyl, 2-Phenoxy	354
32	2105	a	?	41(100) 57(100) 125(73)65(70)56(68) Weak Spectra		
33	2145	a	Phenoxy 1,1'-Biphenyl	77(100)246(66)115(60)51(53)141(31)122(23)		
34	2182	aa	Pentadecylbenzene	Internal Standard	1,1'-Biphenyl, 2-Phenoxy	241
35	2345	aa?	Phosphoric Acid, Triphenyl Ester	77(100)51(53)65(53)96(18)169(13)215(10)	Phosphoric Acid, Triphenyl Ester	502
36	2381	aa	?	57(100)45(90)41(73)36(58)125(32)		
37	2429	a	Subst. Phosphate	77(100)65(39)51(78)91(27)340(15)339(10)		
38	2441	a	Isomer of #15	77(100)322(100)51(35)215(42)226(41)202(38)	Carbonic Acid 4-Methyl Phenyl Methyl Ester	304
39	2440	a	Phthalate	149(100)167(30)55(18)41(16)249(5)	1,2-Benzodicarboxylic Acid Dipentyl Ester	290
40	2489	aa	Tricresyl phosphate	77(100)118(92)117(46)251(35)368(12)31(33)	Benzene Cyclopropyl-	307
41	2516	a	Phthalate, Bis(2-ethylhexyl)	149(100)167(22)37(23)41(23)45(20)	1,2-Benzodicarboxylic Acid Dilauryl Ester	348
42	2540	a	Tricresyl phosphate	77(100)91(62)65(45)165(26)255(20)31(23)	Benzoic Acid, 2-Hydroxy-Phenyl Methyl Ester	234
43	2549	a	Tricresyl phosphate	77(100)51(28)91(28)103(26)251(18)353(13)368(7)	Benzene, (1-Methylethynyl)-	265
44	2594	a	Tricresyl phosphate	91(100)65(50)77(42)165(28)368(25)367(17)368(18)410(5)		
45	2616	aa	Tricresyl phosphate	77(100)353(52)118(61)51(37)91(36)107(32)65(30)	Benzene, (2-Micropropyl)	195
46	2638	a	?	77(100)145(91)160(30)63(27)41(26)115(21)	Benzene, 1-(1,1-Dimethylethyl)-4-Ethynyl-	338
47	2650	a	Tricresyl phosphate	91(100)77(66)65(46)117(39)368(34)79(33)367(20)		
48	2663	a	?	91(100)77(69)165(68)117(51)160(43)45(40)41(30)251(18)		
49	2676	aa	Trilauryl phosphate	145(100)77(75)160(57)251(27)91(25)450(15)		
50	2696	aa	?	77(100)43(46)41(36)91(30)179(23)160(18)		
51	2734	aa	Trilauryl phosphate	91(100)118(95)117(58)103(45)77(38)41(38)43(32)	Benzene, Cyclopropyl	305
52	2757	a	Homolog of #49	145(100)43(50)91(47)160(44)77(44)105(40)107(40)	Naphthalene, 1,2,3,4-Tetrahydro-1,1-Dimethyl-	264
53	2797	aa	Homolog of #49	145(100)77(92)160(78)91(79)103(68)117(68)43(73)	Benzene, (1-Methylethynyl)-	226
54	2804	a	?	145(100)160(46)91(29)115(23)43(23)77(19)	Naphthalene, 1,2,3,4-Tetrahydro-1,8-Dimethyl-	350
55	2855	aa	Homolog of #51	91(100)118(92)43(48)117(63)103(58)77(52)41(48)	Benzene (1-Propyl-1-Homonyl)	217
56	2863	aa	?	145(100)91(63)43(40)160(52)117(48)41(28)115(22)	Naphthalene, 1-Butyl-1,2,3,4-Tetrahydro-1,8-Pentyl	234
57	2868	a	?	145(100)160(43)43(26)91(16)115(12)77(15)	Benzene, 1-(2-Butenyl)-2,3-Dimethyl	359
58	2883	a	Trilaurylbenzyl phosphate	91(100)145(95)43(70)117(61)160(40)283(23)319(20)		
59	2913	aa	?	91(100)43(77)117(61)145(56)160(52)118(50)77(28)		
60	2922	aa				

TABLE A-22. (Continued)

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Element Match	
					Compound	K.I. x 10 ³
61	2972	0	?	43(100) 145(97) 160(68) 91(63) 117(46) 41(40) 77(35) 115(35)		
62	2986	0	?	91(100) 43(81) 103(68) 118(55) 117(56) 77(48) 61(42) 335(30) 319(42)		
63	2995	0	?	43(100) 77(99) 91(87) 115(61) 41(63) 103(55) 187(37) 437(23) 202(30)		
64	3033	0	?	43(100) 145(82) 91(75) 160(52) 117(42) 41(42) 103(33) 118(31)		
65	3060	00	Triethylphenylphosphate	43(100) 145(63) 91(61) 160(42) 117(35) 41(35) 115(22) 105(20)		
66	3101	0	?	145(100) 43(96) 91(78) 160(58) 103(40) 77(38) 41(38)		
67	3113	0	?	91(100) 103(80) 77(62) 43(52) 437(30) 438(15) 41(32) 115(28)		
68	3144	0	?	43(100) 91(61) 187(48) 202(36) 118(31) 41(25) 145(21) 342(6)		
69	3159	0	?	145(100) 43(96) 91(77) 160(53) 319(43) 103(43) 41(36) 77(33)		
70	3205	0	?	43(100) 145(90) 160(65) 91(58) 117(54) 115(28) 105(28)		

TABLE A-23. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 7E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Element Match	
					Compound	K.I. x 10 ³
1	906	00	2-Decoxyethanol	57(100) 41(58) 45(43) 91(32) 75(13) 109(3)		400
3	2181	00	Pentadecylbenzene	Internal Standard		

TABLE A-24. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 8VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13		Air	44(100)
2	0.19	10-100	Dichloromethane	49(100)84(60)
3	0.26	1-10	Chloroform	81(100)85(65)
4	0.26	1-10	Isopropanol	45(100)43(90)41(70)59(4)69(2)
5	0.29	<1	Dichloroethane	62(100)84(30)49(25)98(5)
6	0.38	1-10	Dichloropropane	63(100)41(82)62(70)76(50)
7	0.58	<1	Toluene	91(100)92(60)
8	1.00	~(8)	I.S.	Don't have spectrum.

TABLE A-25. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 8E

GC Peak No.	Retention Index	Amount, μ g/l	Testative Identification	Characteristic Ions in Mass Spectrum	Most Probable Element Match	Ref. No.
1	836	*	Toluene	91(100) 92(68) 65(13) 62(10) 50(7)	Benzene, Methyl	464
2	896	*	3-Hexanone	57(100) 85(50) 41(23) 72(20) 114(13)	3-Heptanone	427
3	915	*	?	85(100) 57(27) 41(77) 43(67) 71(28) 115(23) 131(18)	1,3-Dioxane-2-Propanol, 2-Methyl	206
4	924	*	?	43(100) 85(93) 45(78) 42(52) 58(42) 59(40) 101(13)	Butanoic acid 3-Hydroxy-3-Methyl Ester	267
5	957	*	4-Octanone	57(100) 85(82) 41(48) 142(13)	4-Octanone, 2-Methyl	175
6	983	*	?	69(100) 68(52) 41(43) 54(38) 94(6)	Pentanedinitrile	191
7	1023	*	?	57(100) 41(40) 55(33) 56(32) 83(18)	Hexanol, 2-Ethyl	612
8	1040	*	Acetophenone	105(100) 77(62) 120(22) 51(23) 43(20)	Ethanol, 1-Phenyl	692
9	1137	***	1-Phenyl-1-Propanone	105(100) 77(69) 107(28) 74(22) 134(8)	P-Propanone, 1-Phenyl	530
10	1139	*	?	71(100) 43(86) 41(36) 56(32) 83(30) 173(2)	Hexene, 2,4,5,-Triamethyl	254
11	1155	*	Alcohol C & 11	43(100) 71(96) 56(78) 89(59) 41(50) 145(5) 173(5)	1-Butanol-4-(Hexoxy)-	584
12	1626	*	Alcohol C & 12	73(100) 88(58) 101(46) 55(37) 41(43) 119(28) 174(8)	1,3-Propanediol, 2,2-Dimethyl	224
13	1557	*	Diethyl Phthalate	149(100) 177(18) 176(10) 76(11) 104(8) 105(9) 65(8)	1,2-Benzenedicarboxylic acid diethyl ester	554
14	1682	**	Hexaethylbenzene	Internal Standard		
15	1828	*	Phthalate	149(100) 150(9) 104(8) 37(8) 41(12) 167(3) 223(3)	1,2-Benzenedicarboxylic acid-butyl-2-methylpropyl Ester	596
16	1920	*	Phthalate, Dibutyl	149(100) 150(9) 104(8) 76(5) 41(9) 121(3) 205(2) 223(2)	"	699
17	2035	*	Alcohol	71(100) 43(96) 67(70) 81(70) 137(68) Poor Spectra	Cyclooctadecane, 1,7,11-Triamethyl-4-ethyl-1,7,11-Triamethyl-4-	270
18	2082	*	Alcohol (1-Eicosanol)	43(100) 55(70) 83(70) 97(68) 41(60) 111(26) 125(22)	1-Eicosanol	480
19	2181	**	Pentadecylbenzene	Internal standard		
20	2269	**	Phthalate	149(100) 104(18) 77(12) 57(12) 41(12) 133(11) 207(8) 263(9)	1,2-Benzenedicarboxylic acid, 2-Butoxyethyl Butyl Ester	604
21	2410	*	Alkyl Aromatic-Acetone	105(100) 163(18) 77(27) 207(3)	2,4-Pentanedione 3-Ethyl-3-Hydroxy Benzoin	306
22	2422	*	"	105(100) 162(33) 77(28) 207(2)	"	279
23	2488	*	?	99(100) 105(35) 163(21) 113(18) 211(7)		
24	2512	*	Alkene	55(100) 43(95) 41(93) 69(63) 76(60) 96(53) 97(50) 207(24)	6-Tetralone, Hexamethyl, 7-(Trimethyl Hexyl)	412
25	2606	*	Phthalate	149(100) 112(30) 57(16) 41(16) 207(8) 321(5)	1,2-Benzenedicarboxylic acid, 2-Butoxy, 2-Methyl Butyl Ester	593
26	2744	*	?	59(100) 72(60) 43(50) 55(43)	1,7-Octanediol, 2,7-Dimethyl	303

TABLE A-26. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 9VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13		Air	44(100)
2	0.16	~ 100	Acetone	43(100) 58(30)
3	0.17	1-10	Dichloroethylene	61(100) 63(33) 96(35) 98(22)
4	0.17	10-100	Dichloromethane	49(100) 84(95)
5	0.20	~ 1	2,3-Dimethylbutane	43(100) 42(55) 41(40) 71(30) 86(2)
6	0.21	< 1	3-Methylpentane	57(100) 56(82) 41(70) 43(30)
7	0.23	10-100	Chloroform	83(100) 85(60) 87(10)
8	0.26	< 1	Methylcyclopentane	56(100) 41(50) 69(40) 84(10)
9	0.36	10-100	Bromodichloromethane	83(100) 85(70) 87(10) 127, 129, 131(~ 7)
10	0.55	1-10	Toluene	91(100) 92(60)
11	0.59	1-10	Dibromochloromethane	129(100) 127(80) 131(30) 79, 81(20)
12	1.00	$\sim (8)$	I.S.	75(100) 77(30) 110(25)
13	1.51	< 1	HC NIS2	57(100) 43(73) 71(50) 85(30)
14	1.68	< 1	Isodecane	57(100) 43(70) 71(60) 85(35) H+170
15	1.71	< 1	Alkane	57(100) 43(50) 43(40) 85(15)
16	1.72	< 1	M182 Alkene	69(100) 55(75) 41(55) 57(55) 83(50)

TABLE A-27. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 9E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Mass Spectrometric Element Match	
					Compound	R.I. $\times 10^3$
1	85a	ee	Toluene	91(100) 95(62) 65(13) 61(8) 51(4) 50(3)	Benzene, Methyl	470
2			?	129(100) 127(82) 79(52) 81(31) 131(25) 48(21) 47(20) 93(14)		
3	860	a	?	85(100) 45(54) 55(31) 69(27) 97(13)	Cyclopentadecane, 2,3-Dimethyl	276
4			?	79(100) 81(90) 91(80) 93(54) Poor Spectrum		
5			?	70(100) 83(48) 97(47) 69(40) 98(39) 55(38) 45(22)	2-Cyclohexanol	466
6	887	ee	Chlorocyclohexane	81(100) 79(95) 80(50) 77(40) 53(22) 116(18) 114(15)	Cyclohexane, 2-Chloro	412
7	907	a	?	177(100) 175(64) 179(45) 61(32) 96(26) 95(25) Poor Spectrum		
8	935	/a	Benzaldehyde	105(100) 106(90) 77(55) 51(29) 50(29)	Benzaldehyde	516
9	1002	ee	4-Chlorocyclohexanol	57(100) 80(29) 44(23) 81(21) 134(5) 136(1)	Cyclohexanol, 4-Chloro-, Trans-	329
10	1016	a	2-Chlorocyclohexanone	55(100) 42(71) 132(37) 97(36) 68(35) 88(32)	Cyclohexanone, 2-Chloro-	225
11	1037	eee	Dichlorocyclohexane	81(100) 80(65) 79(26) 41(18) 116(3) 132(1)	Cyclohexane, 1,2-Dichloro-	536
12	1046	a	?	91(100) 45(21) 81(19) 65(17) 92(14)	Benzoicacetic Acid, 2-Propenyl Ester	268
13	1075	ee	2-Bromocyclohexanol	81(100) 57(49) 99(28) 41(23)	Cyclohexanol, 2-Bromo-	444
14	1087	a	Dichlorocyclohexane	81(100) 80(93) 79(60) 53(53) Weak Spectra	Cyclohexane, 1,2-Dichloro-	321
15	1100	a	Undecane	57(100) 43(94) 41(62) 71(52) 56(31)	Heptane, 2,2,4-Trimethyl-	275
16	1115	ee	Bromo-, Chlorocyclohexane	81(100) 79(23) 117(10) 119(4) 198(2) 196(1)	Cyclohexane, 1-Bromo-2-Chloro-, Cis	480
17	1201	a	Dodecane	43(100) 71(86) 57(82) 85(48) 81(45)	2-Tetradecane, 1-Ethoxy-4,4-Dimethyl	407
18	1212	a	?	43(100) 57(91) 71(78) 41(60) 81(25) 98(23)	Hexanal, 5-Methyl-	279
19	1216	a	Dibromocyclohexane	81(100) 127(61) 79(31) 117(22) 128(13)	Cyclohexane, 1,3-Dibromo-	210
20	1265	a	?	97(100) 79(82) 43(58) 132(37) 57(56) 134(155) 115(41)		
21	1280	a	?	57(100) 49(65) 71(64) 41(59) Poor Spectra		
22	1285	a	?	71(100) 57(78) 43(77) 113(20) 112(19) 85(16)	Pentadecane, 2,6,10,14-Tetramethyl	385
23	1290	a	?	97(100) 55(78) 69(77) 40(21) Poor Spectra		
24	1301	a	Tridecane	43(100) 57(91) 71(69) 85(48) 113(7) 112(6)	Dodecane, 2,6,11-Trimethyl-	627
25	1319	a	?	57(100) 71(75) 43(55) 44(50) Poor Spectra		
26	1331	a	Allylcyclohexane	83(100) 55(99) 43(91) 69(81) 57(64) 82(54)	Cyclohexane, Allyl-	310
27	1359	a	?	71(100) 43(99) 57(85) 49(71) 55(63) Weak Spectra		
28	1379	a	?	71(100) 43(72) 57(70) 85(40) 69(26)	Tetradecane, 2,6,10-Trimethyl-	339

TABLE A-27. (Continued)

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Typical Identification	Characteristic Ions in Mass Spectrum	Major Reasonable Source Match	SL # 183
31	1400	0.5	Tetradecane	53(100) 57(85) 71(22) 85(53) 113(41) 132(7)	Tetradecane, 2,6,10-Trimethyl	446
32	1405	0	Branched Hydrocarbon C $\geq$ 14	57(100) 44(70) 43(70) 85(50) 71(13) Weak spectra		
33	1444	0	Branched Hydrocarbon C $\geq$ 14	43(100) 71(93) 57(72) 85(42) 113(20)	Tetradecane, 2,6,10-Trimethyl	423
34	1501	0.1	Pentadecane	57(100) 71(99) 43(92) 85(57) 41(46) 44(39) 69(27) Weak Spectra		
35	1682	0.0	Hexaethylbenzene	Internal standard	1,2-Benzene dicarboxylic Acid, butyl, 2-Naphyl Propyl Ester	561
36	1822	0.1	Phthalate, Dibutyl	149(100) 150(10) 105(4) 76(3) 205(2) 223(1)		
40	2183	0.1	Pentadecylbenzene	Internal standard		
41	2300	0.1	Phthalate, Butyl Benzyl	149(100) 91(50) 123(17) 206(12) 150(15) 132(13)	1,2-Benzene dicarboxylic acid, Dibutyl Ester	208
43	2380	0.1	?	85(100) 125(99) 199(53) 155(48) 133(44)	Octadecane, Hexamethyl-7,12-Bis(3,5,5-Trimethylhexyl)	224
44	2464	0.1	Phthalate	149(100) 167(33) 44(6)		
45	2514	0	Phthalate Bis(2-Ethylhexyl)	149(100) 167(28) 57(12) 43(11) 113(9)		

TABLE A-28. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 9E

GIC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Element Match	E.I. # 103
1	903	44	Toluene	91(100) 92(49) 94(19) 51(6) 50(3)	Benzene, Methyl-	461
3	926	44	?	70(100) 83(52) 55(51) 97(40) 69(41) 43(23) 74(27)	Cyclohexanone, 2-Pyrrol-	398
4	945	44	Pentanoic Acid, 3-Methyl	74(100) 43(57) 59(35) 87(32) 55(20) 99(20) 101(9)	Pentanoic Acid, 3-Methyl-, Methyl Ester	504
7	995	44	Carbitol	45(100) 59(37) 43(28) 72(23) 104(3) 105(2)	Ethane, 1,1'-Oxybis[2-Ethoxy-]	544
11	1031	44	?	87(100) 102(68) 33(37) 41(29) 130(12) 129(11)	Heptanoic Acid, 2-Pyrrol-, Methyl Ester	227
12	1035	4	Dichlorocyclohexane	81(100) 80(60) 79(29) 41(23) 55(20) 62(13)	Cyclohexane, 1,2-Dichloro-, Glc-	395
14	1049	44	Benzoic Acid	105(100) 77(60) 136(22) 51(28) 50(15)	Benzoic Acid, Methyl Ester	576
15	1111	44	Octanoic Acid	74(100) 87(45) 43(41) 41(32) 59(27) 127(11) 105(9) 129(3)	Octanoic Acid, Methyl Ester	446
16	1149	44	Benzoacetic Acid	91(100) 150(29) 85(17) 59(10)		
20	1312	44	Dodecanoic Acid	74(100) 87(63) 43(47) 41(35) 55(29) 143(10) 171(5) 183(2) 185(1)	Dodecanoic Acid, Methyl Ester	504
35	1644	44	p-Toluenesulfonamide	91(100) 155(25) 65(24) 185(21) 121(19)	Benzenesulfonamide, N,4-Dimethyl-	546
36	1710	44	Tetradecanoic Acid	74(100) 87(70) 43(42) 55(30) 143(21) 199(9) 242(2) 243(1)	Tetradecanoic Acid, Methyl Ester	557
40	1809	4	Pentadecanoic Acid	74(100) 87(81) 43(43) 143(23) 213(8)	Pentadecanoic Acid, Methyl Ester	475
41	1875	4	Heptanoic Acid (Br)	156(100) 74(63) 91(33) 157(47) 406(42) 237(40)	Decanoic Acid, Methyl Ester	582
42	1883	4	Fatty Acid C ₁₅	74(100) 87(76) 43(40) 143(20) 129(10)	Hexadecanoic Acid, Methyl Ester	610
43	1914	44	Hexadecanoic acid	74(100) 87(78) 43(48) 55(35) 143(21) 227(5) 271(1)	Heptadecanoic Acid, Methyl Ester	549
48	2010	4	Heptadecanoic Acid	74(100) 87(72) 43(46) 143(20) 221(5) 199(4)	Octadecanoic Acid, Methyl Ester	615
52	2114	44	Octadecanoic Acid	74(100) 87(81) 43(42) 55(34) 143(27) 199(8) 289(6)		
53	2163	4	Impurity ?	63(100) 73(60) 55(52) 60(50) 129(35) 285(8)		
54	2183	44	Pentadecylbenzene	Internal Standard		
55	2224	4	?	43(100) 104(86) 98(68) 117(42) 239(7)	Tetradecanoic Acid, 2-Hydroxyethyl Ester	357
56	2245	4	Alkenoic acid C ₁₈	155(100) 55(48) 87(42) 43(38) 74(32) 109(31) 187(11) 206(3)	Octadecanoic Acid, 9,10-Dihydroxy-	423
57	2255	4	C ₁₈ 19 Alkyl acid	55(100) 74(95)	Cyclopropane Pentenoic Acid, 2-Undecyl-, Methyl Ester, Trans-	372
58	2266	44	Octadecanoic acid 2-Octyl	55(100) 155(68) 43(40) 74(34) 109(27) 97(36)	Octadecanoic Acid, 2-Octyl-, Methyl Ester	546
59	2306	4	Eicosenoic acid	169(100) 87(55) 43(50) 55(42) 74(39) 201(11)	Tetradecanoic Acid, 12-Methyl-, Methyl Ester	295
60	2316	4	Subst. Fatty Acid C ₂₀	74(100) 87(77) 43(55) 143(27) 199(5) 284(6) 327(3)	Hexadecanoic Acid, Methyl Ester	502
61	2429	4	Subst. Fatty Acid C ₂₁	43(100) 104(74) 98(65) 41(54) 117(40) 55(39) 155(12) 154(6)	Eicosenoic Acid, 2-Hydroxy Ethyl Ester	437
62	2451	4	Octadecanoic Acid, 9,10-Dihydroxy	155(100) 87(54) 55(57) 43(47) 74(34) 109(33) 206(6)	Octadecanoic Acid, 9,10-Dihydroxy-, Methyl Ester	494
63	2472	4	Subst. Fatty Acid (unsat.) C ₂₂	74(100) 43(39) 87(33) 55(30)		
64	2480	4	Cloro Fatty Acid	74(100) 43(43) 87(33) 55(31) 95(18) 109(12)	Octadecanoic Acid, 9,10-Dichloro-, Methyl Ester	401

TABLE A-29. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 10VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13		Alf	44(100)
2	0.18	<1	Dichloroethylene	61(100) 96(70) 62(50) 98(42) 47(35)
3	0.19	1-10	Dichloromethane	49(100) 86(100)
4	0.20	<1	Gasole	69(100) 41(60) 40(55) 42(20)
5	0.25	<1	Chloroform	83(100) 95(70)
6	0.27	<1	Tetrahydrofuran	42(100) 41(50) 72(80) 71(30)
7	0.29	<1	Trichloroethane	97(100) 99(70) 61(60) 117, 119, 121 <(10)
8	0.37	<1	Toluene	91(100) 92(60)
9	1.00	<(8)	1,5.	75(100)

TABLE A-30. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 10E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Match	E.I. # 103
1	860	•	7	83(100) 42(68) 41(63) 55(42) 54(41) 69(32) 97(12)	7-Dehalocyclop[4,1,0]heptene	414
2	888	•	7	79(100) 83(56) 69(59) 55(48) 97(63) 98(27) 45(38) 41(26) 78(13)		
3	892	•	7	79(100) 77(33)	Poor spectra	
4	1002	•	HC + Chlorocyclohexene	57(100) 80(76) 41(22) 44(21) 88(13) 98(9) 124(4) 116(3)	Cyclohexene, 4-Chloro-, Trans	227
5	1008	•	7	41(100) 68(58) 43(37) 74(31) 55(25)		
6	1048	•	7	55(100) 41(93) 37(42) 188(33) 81(12)	2-Propenoic Acid, 2-Propenyl Ester	413
7	1134	•	Chlorocyclohexane	79(100) 81(80) 53(60) 41(38) 77(32) 97(25)	Cyclohexene, 2-Chloro-	266
8	1172	•	Bromocyclohexanol	81(100) 127(34) 79(27) 41(26) 57(23) 99(24) 128(10)	Cyclohexanol, 2-Bromo-, Cis-	319
9	1186	•	Dibromocyclohexane	81(100) 41(62) 79(32) 55(30) 57(27) 98(8)		
10	1215	•	Bromochlorocyclohexane	81(100) 127(33) 79(32) 55(21) 41(17) 112(12) 128(8)	Cyclohexane, 1-Bromo-2-Chloro-, Cis-	375
11	1220	•	7	41(100) 80(78) 77(66) 106(65) 159(46) 91(42) 93(35) 161(15)		
12	1387	•	Biphenyl	154(100) 153(43) 152(31) 155(14) 151(11) 76(10)	Acenaphthylene, 1,2-Dihydro-	448
14	1897	•	Allylbenzene	158(100) 112(38) 91(32) 43(27) 159(16) 168(3)	Benzene, 1,3-Bis(1-Methylethanyl)	486
15	2181	•	Pentadecylbenzene	Internal Standard		
•	1679	•	Hexadecylbenzene	Internal Standard		

TABLE A-31. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 10E

GC Peak No.	Retention Index	Amount, µg/l	Testative Identification	Characteristic ions in Mass Spectrum	Most Reasonable Element Match Compound	E.L. n 103
1	1137	a	?	79 (100) 33 (90) 81 (63) 41 (52) 46 (41) 77 (32) 97 (26)	Trichloroethane, 1,1,2-trichloroethyl-	402
2	1509	a	?	91 (100) 155 (35) 186 (32) 45 (31) 107 (15) 122 (6)	Benzene, (Ethoxy Methyl)-	427
3	1653	aa	p-Toluenesulfonamide	91 (100) 45 (31) 135 (25) 105 (21) 121 (19)		
4	1672	a	?	143 (100) 103 (96) 135 (86) 165 (73) 77 (41) 202 (36) 168 (28)	Benzene Sulfonamide, n,4-Dimethyl-	543
5	1708	a	Tetradecanoic Acid	74 (100) 87 (72) 143 (20) 199 (8)		
6	1772	a	?	74 (100) 87 (73) 45 (64) 145 (23) 213 (6) 157 (7)	Tetradecanoic Acid, Methyl Ester	472
7	1782	aa	?	184 (100) 91 (86) 103 (85) 135 (69) 202 (54) 165 (43) 211 (6)	Cyclopentane undecanoic Acid, Methyl Ester	447
8	1808	a	Pentadecanoic Acid	74 (100) 87 (77) 43 (61) 59 (27) 143 (21)		
9	1844	a	?	41 (100) 55 (95) 74 (78) 97 (58) 96 (56) 151 (26) 194 (13) 236 (11)	Dodecanoic Acid, Methyl Ester	253
11	1919	a	?	164 (100) 150 (86) 192 (68) 132 (42) 234 (30) 178 (25) 205 (17)	9-Nonadecanoic Acid, Methyl Ester	446
12	2087	a	Octadecanoic Acid	55 (100) 74 (63) 87 (48) 180 (9) 195 (8) 181 (5) 222 (4)		
14	2110	a	Octadecanoic Acid	74 (100) 87 (72) 43 (58) 143 (20) 199 (5) 137 (3)	10-Octadecanoic Acid, Methyl Ester	573
15	2182	aa	Pentadecylbenzene	Internal Standard	Nonadecanoic Acid, Methyl Ester	726
16	2334	a	?	43 (100) 217 (32) 275 (6) 276 (5) Four Spectra		
17	2378	a	?	45 (100) 217 (80) 43 (66) 218 (17) 170 (16) 177 (13)		
18	2513	a	?	118 (100) 117 (81) 91 (67) 77 (58) 170 (47) 171 (38) 181 (15)		
*			Palmitic Acid	Internal Standard		

TABLE A-32. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 11VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Testative Identification	Characteristic ions in Mass Spectrum
1	0.15		Air	44 (100)
2	0.19	~10	Dichloromethane	84 (100) 49 (95)
3	0.20	1-10	Carbon disulfide	76 (100) 78 (10)
4	0.26	1-10	Chloroform	85 (100) 95 (70)
5	0.27	1-10	Diisopropyl ether	45 (100) 43 (60) 87 (30) 59 (15)
6	0.34	10-100	Carbon tetrachloride	117 (100) 119 (95) 121 (30) 82 (28)
7	0.39	10-100	Dichloropropane	63 (100) 62 (68) 76 (40) 41 (32)
8	1.00	-(8)	I.S.	75 (100) 77, 110 (33)

TABLE A-33. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 12VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum
1	0.13	---	Air	44(100)
2	0.18	10-100	Acetone	43(100) 58(30)
3	0.18	1-10	+ Fluorotrichloroethane	101(80) 103(50) 105(10)
4	0.19	<1	Diethyl ether +	59(100) 45(95) 74(55) 41(55) 76(25) 78(10)
5	0.19	<1	Chloropropene	
6	0.19	1-10	Dichloroethylene	61(100) 86(50) 98(40) 83(30)
7	0.19	1-10	Dichloromethane	49(100) 84(80)
8	0.20	1-10	Carbon disulfide	76(100) 78(15)
9	0.23	<1	2,3-Dimethylbutane	43(100) 42(50) 41(35) 71(20)
10	0.23	<1	Methylethyl ketone	43(100) 72(25)
11	0.24	<1	3-Methylpentane	57(100) 56(95) 41(88)
12	0.25	1-10	Chloroform	83(100) 85(60)
13	0.27	1-10	Tetrahydrofuran	42(100) 41(40) 71(30) 72(30)
14	0.28	1-10	Dichloroethane	62(100) 64(32) 49(30) 98(5)
15	0.29	<1	1,1,1-Trichloroethane	97(100) 99(70) 81(40) 119(15)
16	0.31	1-10	Benzene	78(100)
17	0.37	1-10	1,2-Dichloropropane	63(100) 62(72) 41(68) 76(40)
18	0.37	<1	3-Pentanone	57(100) 86(20)
19	0.38	<1	Bromodichloromethane	83(100) 85(65) 129(10) 127(8) 131(3)
20	0.38	<1	Trichloroethylene	95(100) 130(90) 132(88) 97(70)
21	0.54	1-10	1,1,2-Trichloroethane (T)	97(100) 83(60) 99(70) 81(40) 85(50) 83(25) (Weak)
22	0.56	1-10	Toluene	91(100) 92(60)
23	0.88	<1	C ₂ Alkyl benzene	91(100) 104(30)
24	0.91	<1	C ₂ Alkyl benzene	91(100) 104(40)
25	0.98	<1	C ₂ Alkyl benzene	91(100) 104(40)
26	1.00	~(8)	1,5-	75(100) 77(33) 110(30)
27	1.06	<1	Alkane	71(100) 43(40) 57(55)
28	1.06	<1	Alkane	43(100) 57(90)
29	1.17	<1	C ₃ Alkyl benzene	105(100) 120(20)
30	1.18	<1	C ₃ Alkyl benzene	105(100) 120(20)

TABLE A-33. (Continued)

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Positive Identification	Characteristic Ions in Mass Spectrum
31	1.19	<1	C ₇ Alkyl benzene	105(100) 120(40)
32	1.20	<1	C ₁₀ Branched alkane	57(100) 85(65) 41(40) 142 M
33	1.21	<1	C ₇ Alkyl benzene	105(100) 120(30)
34	1.22	<1	Branched alkane	57(100) 56(35)
35	1.25	<1	C ₇ Alkyl benzene	105(100) 120(35)
36	1.26	<1	Dichlorobenzene	146(100) 148(70)
37	1.27	<1	Branched alkane	57(100) 56(40)
38	1.30	<1	C ₇ Alkyl benzene	105(100) 120(35)
39	1.37	<1	C ₈ Alkyl benzene	105(100) 134(20)
40	1.38	<1	C ₈ Alkyl benzene	119(100) 134(25)
41	1.40	<1	C ₈ Alkyl benzene	105(100) 134(15)
42	1.42	<1	C ₈ Alkyl benzene	119(100) 134(25)
43	1.53	1	C ₉ Alkyl benzene	119(100) 134(20)

TABLE A-34. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 12E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Terminology Identification	Characteristic ions in Mass Spectrum	Most Plausible Isomer Made	R.I. ± 10
2	860	..	Branched hydrocarbon C ≥ 8	57 (100) 85 (26) 41 (21) 43 (20) 72 (13)	Pentane, 2,2-dimethyl-	490
3	887	..	Alkyl Ketone	85 (100) 53 (92) 58 (63) 45 (56) 115 (22) 161 (21)	2-Pentanone, 5-methyl-	305
4	892	..	..	43 (100) 45 (79) 85 (68) 78 (41) Poor MS	1,3,2-Trifluoro, 2,4,6-trimethyl-	215
5	935	..	..	57 (100) 105 (83) 85 (80) 41 (52) 126 (32) 93 (23) 63 (28)	Ethanol, 1-phenyl-	440
9	1042	..	Acetophenone	105 (100) 77 (45) 43 (22) 120 (15)	Undecane	775
15	1099	..	Undecane	43 (100) 57 (22) 71 (41) 85 (30) 136 (2)	Benzene, Methanol, Alpha-Ethyl-	650
18	1136	..	Benzene, Methanol, 4-ethyl	105 (100) 107 (65) 77 (58) 79 (42) 136 (12) 136 (4)	1-Propene, 1-phenyl-	542
18a	1136	..	1-Phenyl 1-Propene	105 (100) 77 (41) 136 (12) 51 (11)	Undecane, 2,4-dimethyl-	631
22	1160	..	HC + Naphthalene	128 (100) 126 (32) 127 (31)	Dodecane, 2,4-dimethyl-	292
23	1164	..	Branched Hydrocarbon C ≥ 11	43 (100) 71 (71) 57 (57) 85 (50) 126 (15)	Benzene, 1-ethyl-3-(1-methyl ethyl)-	476
24	1170	..	Branched Hydrocarbon C ≥ 11	133 (100) 97 (51) 119 (37) 148 (30) 55 (28) 56 (24)	Pentadecane, 5-methyl-	487
26	1182	..	Alkyl Benzene C3	43 (100) 57 (71) 71 (65) 85 (59) 97 (54)	Dodecane	810
27	1187	..	Branched Hydrocarbon C ≥ 11	43 (100) 57 (62) 71 (36) 85 (35) 170 (2)	Tridecane, 4,8-dimethyl-	440
29	1201	..	Dodecane	43 (100) 57 (98) 71 (41) 85 (22) 98 (18) 112 (13) 113 (12) 133 (11)	Tetradecane, 1-chloro	238
31	1216	..	Branched Hydrocarbon C ≥ 12	41 (100) 119 (84) Poor MS	1,2,3,4-Tetrahydro-6-methyl-naphthalene	441
32	1223	..	Branched Hydrocarbon C ≥ 12	131 (100) 118 (58) 146 (53) 105 (38) 91 (32) Good MS	Undecane, 2,4-dimethyl-	309
36	1240	..	Tetrahydro, Methyl-Naphthalene	43 (100) 85 (66) 57 (55) 133 (21) 147 (11)	Dodecane, 2-methyl	493
37	1249	..	Branched Hydrocarbon C ≥ 12	43 (100) 71 (60) 85 (78) 57 (37)	Nonane, 2-methyl-	561
38	1254	..	Branched Hydrocarbon C ≥ 12	64 (100) 57 (69) 85 (62) 71 (36) 99 (18) 113 (10) 141 (8) 140 (7)	Undecane, 2,6-dimethyl-	526
39	1259	..	Branched Hydrocarbon C ≥ 12	142 (100) 141 (80) 57 (67) 115 (51) 85 (40) 71 (36)	Undecane, 3,4,5-trimethyl-	292
40	1265	..	Methyl naphthalene	43 (100) 57 (90) 71 (79) 84 (13) 85 (10)	Tetradecane, 2,5-dimethyl-	257
41	1270	..	Branched Hydrocarbon C ≥ 12	142 (100) 141 (93) 115 (60) 143 (13) 145 (10)	Hepadecane, 2,6,10,16-tetramethyl-	223
43	1279	..	Branched Hydrocarbon C ≥ 12	43 (100) 57 (62) 85 (37) 71 (35) 184 (2)	Tetradecane, 4,11-dimethyl	503
47	1301	..	Tridecane	43 (100) 71 (98) 83 (41) 56 (37) 131 (19) 147 (9)	Nonane, 2,2,6,6,6-penta-methyl-	250
56	1349	..	Branched Alkane C ≥ 13	43 (100) 57 (91) 85 (71) 71 (57) 105 (34) 154 (27)		
55	1351	..	Branched Hydrocarbon C ≥ 13	Poor MS		
56	1353	..	Branched Hydrocarbon C ≥ 13	43 (100) 71 (61) 57 (69) 85 (43) 99 (22) 145 (12)		
57	1358	..	Branched Hydrocarbon C ≥ 13	63 (100) 57 (52) 85 (38) 71 (36) 99 (18) 113 (12) 155 (7)		
58	1363	..	Branched Hydrocarbon C ≥ 13	63 (100) 57 (52) 85 (38) 71 (36) 99 (18) 113 (12) 155 (7)		
59	1370	..	Branched Hydrocarbon C ≥ 13	63 (100) 57 (52) 85 (38) 71 (36) 99 (18) 113 (12) 155 (7)		

TABLE A-34. (Continued)

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Element Made	R.I. ± 10
60	1376	uv	Alkyl naphthalene, C ₂	156 (100) 141 (67) 155 (33) 115 (20) 95 (12) 157 (11)	Naphthalene, 1,4-Dimethyl-	258
62	1392	u	Alkyl naphthalene, C ₂	156 (100) 141 (83) 83 (72) 80 (46) 101 (41) 157 (12)		
63	1400	uv	Tetradecane	43 (100) 57 (63) 85 (50) 71 (45)	Tetradecane	616
72	1443	u	Branched Hydrocarbon C ≥ 14	43 (100) 71 (59) 57 (54) 85 (49) 99 (21) 113 (18) 141 (16)	Dodecane, 2-Methyl-	447
73	1470	u	Branched Hydrocarbon C ≥ 14	57 (100) 43 (63) 85 (61) 71 (58) 99 (27)	Tetradecane, 2,5-Dimethyl-	453
77	1501	pu	Pentadecane	43 (100) 57 (65) 85 (52) 71 (52) 99 (13) 170 (1)	Dodecane, 2,6,11-Trimethyl-	632
82	1548	u	Hexadecane	43 (100) 57 (77) 71 (62) 85 (52) 99 (15) 127 (7)	Hexadecane	581
84	1680	uv	Hexamethylbenzene	Internal Standard		
85	1698	u	Heptadecane	56 (100) 43 (93) 71 (80) 85 (61) 61 (59)		
86	2181	uv	Pentacyclononene	Internal Standard		

TABLE A-35. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 12E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum	Most Plausible Benzenic Match Compound	R.I. ± 10
4	987	66	Carbitol	45 (100) 59 (33) 75 (25) 104 (3) 103 (2)	Ethanol, 2-(2-ethoxy ethoxy)-	565
8	1167	6	2-hydroxy Benzoic Acid	120 (100) 92 (86) 152 (6) 121 (3) 165 (48) 163 (22)	Benzoic Acid, 2-hydroxy-Methyl Ester	228
9	1187	6	Benethiadiazole	135 (100) 108 (41) 69 (31) 82 (15) 63 (13) 136 (9) 91 (8)	1,2,3-Benzethiadiazole	373
10	1377	6	?	71 (100) 43 (73) 97 (17) 172 (3) 172 (2)	Myricic Acid, Thio-, 5-Decyl Ester	227
11	1509	6	Dodecanoic Acid	74 (100) 87 (61) 43 (32) 55 (30) 59 (20) 143 (11) 171 (7)		
12	1554	6	?	101 (100) 146 (86) 108 (60) 69 (38) 45 (39) 136 (27) 180 (25)		
14	1885	6	Tetradecanoic Acid	74 (100) 87 (61) 43 (35) 55 (29) 59 (18) 143 (13)		
15	1913	66	Subst. Fatty Acid C ≥ 15	55 (100) 74 (70) 96 (44) 87 (34) 181 (15) Poor MS		
16	1921	6	Hexadecanoic Acid	Internal Standard		
19	1982	6	Phthalate, Dibutyl	149 (100) 41 (14) 78 (12) 104 (11) 105 (10) 150 (9) 223 (2)	1,2-Benzenebis(carboxylic Acid, Dibutyl Ester)	219
22	2073	6	Subst. Fatty Acid C ≥ 16	74 (100) 87 (63) 43 (32) 55 (30) 41 (27) 143 (19) 185 (13)		
23	2083	6	9,12-Octadecadienoic Acid	67 (100) 81 (79) 55 (61) 95 (57) 45 (52) 79 (51) 104 (31)	9,12-Octadecadienoic Acid, Methyl Ester	346
26	2114	6	Octadecanoic Acid	55 (100) 41 (88) 43 (67) 69 (60) 74 (52) 83 (41) 1265 (11) 17	10-Octadecanoic Acid, Methyl Ester	340
27	2121	6	Octadecanoic Acid	74 (100) 87 (67) 43 (53) 55 (37) 41 (30) 145 (10)	Heptacosanoic Acid, Methyl Ester	710
28	2131	6	Phenyl subet. Acid	91 (100) 105 (66) 77 (64) 115 (62) 119 (60) 232 (19) 199 (10)		
29	2139	6	"	91 (100) 146 (87) 133 (81) 105 (82) 101 (75) 141 (61)		
31	2183	66	Pentadecyl Benzeno	146 (100) 91 (55) 117 (54) 133 (51) 109 (33) 105 (30)		
32	2170	66	Subet. Benzoic Acid	Internal Standard		
33	2196	6	?	91 (100) 105 (82) 79 (63) 41 (64) 241 (19) 202 (2)	2,5-Octadecadienoic Acid, Methyl Ester	375
34	2210	6	?	121 (100) 91 (38) 105 (32) 243 (5) 244 (3) 304 (2) Good MS		
37	2248	6	?	121 (100) 91 (38) 105 (32) 79 (25) 55 (20)		
38	2267	6	?	43 (100) 41 (63) 55 (52) 261 (11) 305 (3)		
39	2275	6	?	121 (100) 91 (67) 79 (58) 81 (54) 105 (55) 107 (54) 215 (17) 241 (8) 237 (2)		
41	2306	66	Chloroalkylphenyl Acid	91 (100) 41 (99) 43 (98) 105 (80) 55 (68) 79 (57) 131 (54) 213 (14) 243 (13) 241 (12) 215 (6)		
43	2366	66	Alkyl subet. benzoic acid	43 (100) 91 (78) 121 (75) 105 (62) 243 (22) 215 (13) 306 (6)		
45	2355	66	Subet. Benzoic Acid	105 (100) 91 (90) 121 (80) 43 (51) 185 (37) 213 (31) 257 (11) 256 (10) 317 (4)		
46	2373	6	"	105 (100) 91 (99) 131 (70) 43 (60) 78 (57) 146 (51) 213 (15) 303 (5)		
47	2388	66	?	109 (100) 43 (91) 95 (88) 67 (68) 91 (62) 217 (35) 261 (29) 305 (11)		
55	2487	6	?	43 (100) 237 (78) 129 (67) 41 (63) 59 (60) 255 (14)		
58	2524	6	?	128 (100) 59 (90) 253 (83) 115 (82) 187 (76) 91 (52) 269 (9)		
65	2807	66		Internal Standard		

TABLE A-36. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 13VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13		Air	44(100)
2	0.16	<1	Dichloromethane	49(100)86(60)
3	0.16	<1	Carbon disulfide	76(100)
4	0.18	10-100	Dichloromethane	49(100)86(60)
5	0.18	~10	Carbon disulfide	76(100)
6	0.26	10-100	Chloroform	83(100)85(70)
7	0.31	10-100	Carbon tetrachloride	117(100)119(95)82(30)
8	0.35	1-10	1,2-Dichloropropane	63(100)62(70)76(40)
9	0.36	1-10	Bromodichloromethane	83(100)85(70)127(10)139(15)
10	0.55	1-10	Toluene	91(100)92(50)
11	1.00	-(8)	I.S.	75(100)110(50)

TABLE A-37. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 14VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12		Air	44(100)
2	0.13	1-10	Vinyl formate or Acetaldehyde	44(100)43(80)42(25)
3	0.16	1-10	Dichloromethane	49(100)84(90)
4	0.18	<1	Dichloroethylene	61(100)96(40)98,63(30)
5	0.19	<1	2,3-Dimethylbutane	44(100)43(50)42(30)71(20)
6	0.20	<1	3-Methylpentane	57(100)56(95)41(90)71(5)86(4)
7	0.21	<1	N,N-Dimethylformamide (T)	73(100)44(65)45(30)128,130(2)
8	0.21	1-10	Chloroform	83(100)85(70)
9	0.24	<1	Methyl cyclopentane	56(100)41(60)69(40)84(6)
10	0.25	~10	2-Methyl-1,3-dioxolane	73(100)43(90)45(70)58(30)87(10) Big Peak
11	0.35	<1	1,4-Dioxane	88(100)58(93)43(45)
12	0.55	<1	Toluene	91(100)92(50)
13	1.00	-(8)	I.S.	75(100)
14	1.30	<1	Alkane ($\text{C}_{10}\text{H}_{20}$)	57(100)43(80)71(40)

TABLE A-38. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 14E

GC Peak No.	Retention Time	Amount, μ g/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Match	K.I. $\times 10^3$
1	856	*	Methylcyclohexane	83(100)55(98)96(50)	Cyclohexane, Methyl-	599
2	861	*	Toluene	92(100)91(98)65(34)	Benzene, -Methyl	569
3	1148	*	H,H-Dimethylacetamide	44(100)87(55)72(20)	Acetamide, H,H-Dimethyl	869
4	1354	***	1,1'-Alphenyl	154(100)153(65)76(55)132(45)11(30)63(25)	1,1'-Alphenyl	638
5	1376	***	Diphenyl Ether	170(100)31(100)77(95)154(92)141(73)	Benzene, 1,1'-Diphenyl	559
6	1477	*	Dibenzofuran	168(100)139(50)89(20)169(18)	Dibenzofuran	455
7	1641	*	1,4-Methanaphthalene-8-ol, 1,4-Dihydro-	157(100)128(70)129(42)77(31)138(10)	1,4-Methanaphthalene-8-ol, 1,4-Dihydro-	513
8	1808	*	H,4-Dimethylbenzenesulfonamide	91(100)65(32)185(16)155(18)	Benzenesulfonamide, H,4-Dimethyl	649
9	1920	*	Dibutyl Phthalate	149(100)41(15)150(10)205(3)223(5)	1,2 Benzenedicarboxylic Acid, Butyl 2-Methylpropyl Ester	587

TABLE A-39. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 15VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.10		Air	44(100)
2	0.10	10-100	Carbonyl sulfide	60(100)62(5)
3	0.13	1-10	Dichloroethylene	61(100)96(70)
4	0.13	10-100	Dichloromethane	84(100)49(95)
5	0.14	10-100	Carbon disulfide (lots)	76(100)44(75)78(35)
6	0.18	10-100	Chloroform	83(100)85(90)
7	0.20	1-10	1,2-Dichloroethane	62(100)49(32)64(30)
8	0.21	1-10	1,1,1-Trichloroethane	97(100)99(70)117,119(20)
9	0.23	1-10	Benzene	78(100)
10	0.23	10-100	Carbon tetrachloride	117(100)119(98)82(30)
11	0.27	10-100	1,2-Dichloropropane	63(100)62(70)76(40)
12	0.27	1-10	3-Pentanone	57(100)86(20)
13	0.28	10-100	Bromodichloromethane	83(100)85(70)127,129,131
14	0.44	1-10	Toluene	91(100)
15	0.48	1-10	Dibromochloromethane	129(100)127(80)208,210
16	0.59	1-10	1,1,1,2-Tetrachloroethene	129(100)166(95)131(90)166(80)
17	1.00	-(8)	I.S.	75(100)
18	1.15	1-10	Butyl ketone (T)	85(100)57(98)100,127(-8)
19	1.17	1-10	Alkane C_8H_{18}	57(100)71,43,85,99

TABLE A-40. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 15E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Molecular Weight	
					Compound	E.I. $\times 10^3$
1	862	++	oxa bicyclo [4.1.0] heptene	83 (100) 41 (72) 42 (70) 54 (69) 69 (35) 97 (17) 98 (4)	7-Oxabicyclo [4.1.0] heptene	578
2	881	++	Cyclohexanol	70 (100) 83 (38) 90 (37) 91 (31) 97 (25) 98 (20)	2-Cyclohexen-1-ol	608
3	890	++	Chlorocyclohexane	81 (100) 79 (61) 80 (35) 93 (27) 77 (22)	Cyclohexene, 3-Chloro-	612
4	932	*	Dimethylpentanol	57 (100) 85 (70) 91 (42) 98 (27)	Pentanol, 2,3-dimethyl	621
5	1006	++	?	69 (100) 68 (47) 91 (39) 92 (26) 54 (28)	Cyclopentane, Chloro-	319
6	1035	+++	Chlorocyclohexanol	57 (100) 80 (25) 88 (11) 90 (4) 134 (3) 136 (1)	Cyclohexanol, 4-Chloro	530
7	1074	++	?	71 (100) 41 (18) 81 (13) 97 (12) poor spectrum		
8	1101	+++	Dichlorocyclohexane	81 (100) 80 (56) 91 (17) 88 (4) 90 (3) 114 (2) 118 (1)	Cyclohexane, 1,2-dichloro-, Cl-	595
9	1113	+++	Bromo-cyclohexanol	81 (100) 57 (78) 99 (23) 91 (22) 132 (3) 134 (3)	Cyclohexanol, 2-Bromo-, Cl-	576
10	1121	++	Bromomethoxycyclohexane	71 (100) 81 (66) 91 (28)	Cyclohexane, 1-Bromo-2-Methoxy-Cl-	438
11	1124	++	Bromochlorocyclohexane	81 (100) 41 (10) 53 (9) 117 (8) 119 (2)	Cyclohexane, 1-Bromo-2-Chloro, Cl-	521
12	1133	++	1-Phenylpropanone	105 (100) 77 (65) 51 (25) 134 (12)	1-Propanone, 1-Phenyl	656
13	1140	*	1-Phenylpropanol	77 (100) 79 (82) 105 (92) 107 (92) 51 (41) 134 (10) 136 (8)	Benzene Methanol, α -ethyl-	457
14	1215	*	Dibromocyclohexane	81 (100) 41 (19) 161 (6) 163 (6)	Cyclohexane, 1,3-dibromo-	641
15	1386	*	Hexyloxybutanol	71 (100) 56 (81) 93 (77) 89 (33)	1-Butanol, 4-(Benzoyloxy)-	613

TABLE A-41. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 16VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Testane Identification	Characteristic Ions in Mass Spectrum
1	0.14		Air	
2	0.19	<1	Dichloromethane	49(100)84(50)
3	0.29	<1	1,1,1-Trichloroethane	97(100)61(70)99(60)112,114,116
4	0.39	1-10	Trichloroethylene	95(100)130(80)132(78)97(70)40(60)
5	0.91	1-10	C ₂ Alkyl benzene	91(100)106(45)
6	1.00		1,5-	75(100)
7	1.26	1-10	C ₃ Alkyl benzene	105(100)120(40)
8	1.43	1-10	C ₄ Alkyl benzene	119(100)
9	1.50	1-10	C ₅ Alkyl benzene	119(100)

TABLE A-42. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 17VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Testane Identification	Characteristic Ions in Mass Spectrum
1	0.11		Air	
2	0.14	<1	Trichlorotrifluoro ethane	101(100)103(70)131(60)133(40)
3	0.15	1-10	Dichloroethylene	96(100)61(80)98(70)59(40)
4	0.15	1-10	Dichloromethane	49(100)
5	0.16	1-10	Trichlorotrifluoroethane	131(100)101(70)133(60)103(50)
6	0.18	1-10	2,3-Dimethylbutane	43(100)42(52)41(45)71(35)
7	0.20	1-10	3-Methylpentane	57(100)56(88)41(70)
8	0.21	10-100	Chloroform	83(100)
9	0.24	<1	Methyl cyclopentane	58(100)41(60)69(40)84(6)
10	0.25	<1	1,1,1-Trichloroethane	97(100)99(70)61(45)112,114,116
11	0.35	<1	Trichloroethylene	95(100)132(95)130(92)
12	0.56	1-10	1,3-Dioxane	91(100)

TABLE A-43. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 18VI

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.16	<1	Acetone	43(100) 58(30)
3	.16	<1	Diethyl ether	59(100) 74(73) 45(65)
4	.17	<10	Dichloromethane	49(100) 84(40)
5	.23	<1	Chloroform	83(100) 95(67)
6	.25	<1	Tetrahydrofuran	42(100) 72(32) 71(30)
7	.27	<1	1,1,1-Trichloroethane	97(100) 61(70) 99(65)
8	.29	<1	Benzene	78(100)
9	.36	<1	Trichloroethylene	130(100) 95(87) 132(75) 97(70)
10	.54	<1	Toluene	91(100) 92(60)
11	.68	<1	1,1,2,2-Tetrachloroethane	166(100) 129(92) 164(82) 131(70)
12	1.00	-(8)	T.S.	75(100) 77(13)

TABLE A-44. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 18VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.14		Air	44(100)
2	0.18	1-10	Dichloroethylene	61(100) 96(62) 98(40)
3	0.18	10-100	Dichloromethane	49(100)
4	0.25	1-10	3-Methylpentane + Chloroform	41(100) 57(92) 83(80) 43(70)
5	0.29	1-10	1,1,1-Trichloroethane	97(100) 99(70) 117, 119, 121
6	0.31	<1	Benzene	78(100)
7	0.57	1-10	Toluene	91(100)
8	1.00	1-10	T.S.	75(100)

TABLE A-45. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 18E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Monomer Match	
					Compound	E.I. m/z
1	948	**	Carbitol	45(100)59(35)72(27)104(4)103(3)	Ethane, 1,1'-Oxybis[2-Ethoxy-	618
2	1076	**	?	66(100)91(14)87(13)121(5)132(4)		
3	1083	**	?	66(100)91(12)87(10)121(5)122(4)		
4	1233	**	Dimethylhydrosymethoxy benzaldehyde + ?	137(100)83(99)109(51)53(46)180(44)		
5	1241	*	Dichlorobenzoic acid	173(100)172(66)143(39)109(24)74(22)204(20)206(12)207(4)	Benzoic acid, 3,4-Dichloro, methyl ester	374
6	1442	**	Indolinocarboxyaldehyde, hydroxy methyl	177(100)165(36)131(32)91(29)178(12)		
7	1506	*	Dodecanoic acid	74(100)87(68)	Dodecanoic acid, methyl ester	318
8	1708	**	Tetradecanoic acid + ?	74(100)87(71)158(83)143(19)211(2)	Tetradecanoic acid, methyl ester	329
9	1749	**	?	140(100)183(76)113(20)83(8)		
10	1779	**	C ≥ 13 Fatty acid	74(100)87(71)143(18)199(14)236(0.1)	Tetradecanoic acid, 1,3-Dimethyl-, methyl ester	706
11	1791	**	C ≥ 15 Fatty acid + ?	133(100)132(61)74(30)87(20)212(18)		
12	1836	**	?	198(100)173(32)115(29)129(27)213(21)171(22)76(15)		
13	1864	**	C ≥ 16 Fatty acid	55(100)41(71)74(66)87(64)236(2)	9-Hexadecanoic acid, methyl ester, (E)-	487
14	1910	**	Hexadecanoic acid	71(100)87(72)43(27)35(24)143(19)270(2)	Hexadecanoic acid methyl ester	672
15	1990	*	C ≥ 16 Fatty acid	55(100)69(60)74(55)87(32)137(26)199(13)	13-Octadecanoic acid, methyl ester	321
16	2085	*	C ≥ 18 Fatty acid	55(100)69(65)74(57)87(42)199(17)222(4)	11-Octadecanoic acid, methyl ester	382
17	2111	*	Octadecanoic acid	74(100)87(60)55(28)143(26)235(3)	Hexadecanoic acid, methyl ester	607

TABLE A-46. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 18E

QC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Lines in Mass Spectrum	Most Reasonable Minimum Match Compound	Ref. #
1	865	oo	Methylcyclopentanone	53(100)81(86)67(56)56(41)(26)95(6)9.7(4)	2-Cyclopenten-1-one, 2-Methyl	700
2	1036	oo	Methylpyridine + ?	93(100)66(51)94(10)	Pyridine, 3-Methyl	426
3	1126	oo	Benzoic acid + ?	128(100)102(20)121(17)127(18)63(10)129(10)		
4	1143	oo	Isosquinoline	129(100)102(20)121(17)127(18)63(10)129(10)	Isosquinoline	561
5	1193	oo	1,4-Naphthylidene	130(100)129(26)76(20)103(26)104(23)79(19)50(20)131(9)	1,4-Naphthylidene	683
6	1210	oo	1,2-Benzisothiazole C ₇ H ₅ S ₂	135(100)108(20)91(13)82(13)63(12)45(11)136(18)131(9)	1,2-Benzisothiazole	458
7	1239	oo	3-Methylisoxazole C ₄ H ₅ O ₂	115(100)116(44)144(44)135(20)63(20)89(15)	Cinnoline, 3-Methyl	394
8	1246	oo	Methylisophthalene + ?	141(100)142(82)115(74)130(70)76(25)103(24)		
9	1271	oo	Methylisophthalene	144(100)143(42)117(25)145(10)		
10	1290	ooo	Methylisoxazole	115(100)144(51)116(42)89(12)63(13)50(10)	1,4-Naphthylidene	723
11	1300	oo	Methylisoxazole C ₁₂ H ₁₁	143(100)115(76)116(42)89(12)63(13)146(18)	Cinnoline, 3-Methyl	525
12	1313	oo	Methylisoxazole	115(100)144(54)116(42)89(12)63(13)146(18)	Isosquinoline, 1-Methyl	478
13	1329	o	Dimethylisophthalene	158(100)137(36)143(18)130(13)89(9)63(10)139(11)	Cinnoline, 3-Methyl	552
14	1350	oo	Mixture ? M ₁ M ₂	129(100)147(96)115(78)165(48)91(42)77(32)50(28)	1,4-Naphthylidene	476
15	1401	oo	Pyridine[2,3-b]Pyridine Dimethyl C ₁₀ H ₁₀ N ₂	131(100)145(86)132(78)145(40)63(20)51(18)104(19)118(16)	1H-Pyridine[2,3-b]Pyridine, 2-Ethyl	555
16	1427	oo	Methylbenzimidazole	131(100)132(80)104(18)77(19)51(16)133(7)	Pyridine[2,3-b]Pyridine	382
17	1496	oo	Dimethylbenzimidazole + Carbazole	146(100)145(98)167(45)77(27)104(24)131(22)51(20)166(14)168(4)		
18	1530	oo	Dimethylbenzimidazole + ? C ₁₀ H ₁₀ N ₂	146(100)145(98)167(45)77(27)104(24)131(22)51(20)166(14)168(4)		
19	1540	oo	C ₁₂ -Benzimidazole + ?	145(100)140(68)159(51)146(47)167(16)91(18)77(16)51(14)	1H-Benzimidazole, 5,6-Dimethyl	442
20	1579	oo	Phenanthroline C ₁₂ H ₉ N ₂	180(100)153(67)178(24)152(18)186(16)63(10)181(11)		
21	1596	oo	Benzoic acid + methylisoxazole C ₁₃ H ₁₁ O ₂	165(100)154(97)166(28)195(16)139(12)126(11)65(10)	Benzoic acid, 4-Methyl	446
22	1903	o	Mixture ?	108(100)141(20)116(19)140(22)113(12)63(8)169(13)	9H-Pyridine[3,4-b]Indole	399
23	2472	oo	?	117(100)131(16)141(18)116(14)203(4)		

TABLE A-47. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 19VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	--	Air	44(100)
2	0.16	10-100	Acetone	43(100)
3	0.23	1-10	Chloroform	83(100)
4	0.26	<1	1,1,1-Trichloroethane	97(100)99(70)61(30)117,119,121
5	0.35	<1	Bromodichloromethane	83(100)85(70)127,129,131
6	0.40	<1	Dibromochloromethane	129(100)127(80)131(30)75,81
7	1.00	-(8)	1.S.	75(100)

TABLE A-48. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 20VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	--	Air	44(100)
2	0.19	10-100	Dichloromethane	49(100)
3	0.23	1-10	3-Methylpentane	57(100)56(85)41(70)71(5)
4	0.25	10-100	Chloroform	83(100)
5	0.28	<1	Tetrahydrofuran	42(100)41(45)71,72(30)
6	0.29	10-100	Methyl cyclopentane	56(100)69(50)4(2)84(5)
7	0.30	1-10	1,1,1-Trichloroethane	97(100)99(70)61(50)117,119,121
8	0.40	1-10	Bromodichloromethane	83(100)85(70)127,129,131
9	1.00	1-10	1.S.	75(100)
10	1.37	10-100	C ₇ Alkyl benzene	105(100)119(80)134(20)
11	1.38	1-10	C ₇ Alkyl benzene	105(100)
12	1.39	1-10	C ₇ Alkyl benzene	105(100)
13	1.65	10-100	M126 Alkene C ₉ H ₁₈	43(100)55(80)69(60)83,97,111

TABLE A-49. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 21VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum
1	0.12		Air	44(100)
2	0.16	10-100	Acetone	43(100) 58(30)
3	0.17	10-100	Dichloromethane	49(100)
4	0.21	1-10	Methylethyl ketone	43(100) 72(20)
5	0.23	1-10	Chloroform	83(100)
6	0.30	1-10	Benzene	78(100)
7	0.50	10-100	4-Methyl-2-pentanone	43(100) 58(52) 85(13) 100(9)
8	0.56	>10	Toluene	91(100)
9	0.60	10-100	Dibromochloromethane	179(100) 127(75) 208(9)
10	0.88	1-10	C ₂ -Alkyl benzene	91(100)
11	1.00	~(8)	I.S.	75(100)

TABLE A-50. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 21E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum	Most Reasonable Elemental Match
1	853	*	Hexylpentanal	69(100) 41(95) 57(73) 96(18)	Compound
2	864	***	Hexanal	83(100) 56(69) 55(45) 57(35) 40(32) 70(22) 97(12) 98(4)	2-Pentenal, 2-Methyl-
3	884	**	Cyclohexanol	70(100) 83(37) 55(35) 68(31) 41(26) 97(25) 98(22)	7-oxabicyclo[4.1.0] heptane
4	893	**	Chlorocyclohexane	81(100) 79(66) 53(26) 70(38) 116(10) 118(4)	2-Cyclohexanol
5	912	**	Heptalene	177(100) 175(62) 61(36) 60(36) 179(46) 212(7) 214(5) 210(4) 176(4)	Cyclohexene, 3-Chloro-
6	1015	***	Chlorocyclohexanol	57(100) 80(65) 44(45) 81(41) 88(28) 98(18) 136(10) 136(4)	Cyclohexanol, 4-Chloro-, Trans-
7	1044	***	Dichlorocyclohexane	80(100) 81(99) 77(77) 55(47) 100(49) 120(13) 152(3) 154(2)	Cyclohexane, 1,3-dichloro-
8	1086	***	Bromocyclohexanol	57(100) 81(96) 59(41) 27(39) 99(32) 134(5) 178(1) 180(1)	Cyclohexanol, 2-Bromo-, Trans-
9	1118	**	Bromochlorocyclohexane	81(100) 70(36) 41(30) 55(28) 117(20) 118(6)	Cyclohexane, 1-Bromo-2-Chloro, Cis-

TABLE A-51. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 22VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.16		Air	44(100)
2	0.19	>100	Acetone	43(100)
3	0.20	10-100	Dichloromethane	49(100)
4	0.21	10-100	Carbon disulfide	76(100)
5	0.24	1-10	Methylethyl ketone	43(100) 72(20)
6	0.26	1-10	Chloroform	83(100)
7	0.30	1-10	1,1,1-Trichloroethane	97(100) 99(70) 61(30) 112, 114(13)
8	0.51	1-10	4-Methyl-2-pentanone	43(100) 58(30) 85, 100
9	0.57	10-100	Toluene	91(100)
10	0.80	1-10	4-Vinyl cyclohexene	54(100) 78(80) 66(40) 91, 93(20)
11	0.87	10-100	C ₉ Alkene C ₉ H ₁₈	43(100) 57(50) 71(15)
12	0.87	1-10	C ₇ -Alkyl benzene	91(100) 106(45)
13	1.00	--	I.S.	75(100)
14	1.29	1-10	C ₁₀ H ₁₈ , e.g., C ₄ Alkyl cyclohexene	95(100) 67(60) 68(38) 81(32) 41(26) 123(21) 138(15)

TABLE A-52. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 22E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ion in Mass Spectrum	Most Reasonable Reference Match	
					Compound	R.I. ± 10
1	879	ee	Toluene	91(100)95(67)85(19)63(12)	Benzene, Methyl	572
2	922	ee	Methylbenzene	43(100)59(36)71(10)81(4)114(1)	2-Methoxene, 5-Methyl	807
3	973	ee	1-Alkyl-2-oxene C $\geq$ 7	43(100)41(81)89(32)97(36)106(25)78(21)112(18)		
4	1023	ee	Methylcyclohexanone	55(100)56(45)41(50)112(23)83(20)	Cyclohexanone, 4-Methyl	836
5	1042	ee	Methylcyclohexanol	57(100)41(18)58(41)81(40)55(36)70(20)96(13)	Cyclohexanol, 4-Methyl	533
6	1090	ee	C ₇ -Alkylbenzene	43(100)77(92)105(82)51(56)120(19)		
7	1061	ee	1-Methyl-1-Phenylethane	43(100)121(38)77(16)51(16)122(4)	Benzene Methanol, α - β -Dimethyl	708
8	1123	ee	C ₈ -Alkylcyclohexanol	71(100)43(74)81(16)98(13)123(7)141(6)	Cyclohexanol, 1-Methyl-4-(1-Methyl Ethyl)-	453
9	1135	ee	Alkyl-Alcohol C $\geq$ 9	59(100)113(10)123(4)	Triene	
10	1155	ee	C ₈ -Alkylcyclohexanol	71(100)43(69)72(14)	1,8-Dioxanediol, 8-Methyl-	496
11	1164	ee	Alkyl-Alcohol C $\geq$ 9	55(100)41(70)37(43)81(40)83(25)124(17)96(14)109(9)	Cyclohexanol, 4-(1-Methyl Ethyl)-	344
12	1173	ee	Alkyl-Alcohol C $\geq$ 9	55(100)59(86)81(32)95(35)67(47)136(13)	Bicyclo[2,2,1]heptan-2-ol, 1,7,7,-	515
13	1299	ee	Alkyl-2-oxene C $\geq$ 11	43(100)71(82)59(56)112(10)137(4)155(2)	Triamethyl-	
14	1338	ee	Alkyl-Alcohol C $\geq$ 12	43(100)87(81)41(40)69(61)55(56)81(33)97(14)	4,9-Dodecadiene	332
15	1654	ee	Alkylphenol C $\geq$ 13	135(100)107(49)91(14)121(12)149(6)	1,8-Dioxanediol	500
16	1668	ee	Alkylphenol C $\geq$ 13	121(100)58(76)107(50)143(20)177(7)	Phenol, 4-(2,2,3,3-tetra methyl butyl)-	475
17	1696	ee	Nonylphenol C $\geq$ 15	135(100)107(24)41(16)136(10)	Phenol, 3-(1,1-dimethyl Ethyl)	445
18	1705	ee	Nonylphenol C $\geq$ 15	107(100)135(67)149(56)121(55)55(22)77(17)91(16)191(10)	Phenol, Methyl-	656
19	1712	ee	Alkylphenol C $\geq$ 16	107(100)135(66)121(69)91(18)77(19)163(20)177(13)	Phenol, Dodecyl-	421
20	1725	ee	Alkylphenol C $\geq$ 16	107(100)121(68)149(61)77(18)55(18)177(13)		
21	1740	ee	Alkylphenol C $\geq$ 16	135(100)107(44)41(28)121(14)149(12)	Phenol, Methyl-	532

TABLE A-53. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 22E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Molecular Weight	Reference
1	923	oo	Phenol	94 (100) 93 (99) 92 (88) 66 (99) 63 (97) 50 (91) (decarboxylated)	Phenol	203
2	1062	oo	Benzoic acid	136 (100) 105 (100) 77 (96) 51 (97) (decarboxylated)		
3	1162	oo	Methylcyclohexene-1-carboxylic acid	90 (100) 87 (96) 96 (98) 122 (75) 139 (9) 154 (4)	3-Cyclohexene-1-carboxylic acid, 4-methyl	349
4	1169	oo	Methylcyclohexene-1-carboxylic acid	94 (100) 95 (99) 87 (99) 80 (99) 67 (98) 122 (82) 139 (15) 154 (2)	"	266
5	1506	e	Dodecanoic acid	87 (100) 74 (98) 43 (76) 55 (55) 143 (12) 185 (2) 216 (1)		
6	1543	oo	?	58 (100) 41 (97) 109 (80) 136 (54) 168 (52) 140 (30) 224 (4)		
7	1576	ooo	C = 14 Branched fatty acid + Methyl phenol	117 (100) 59 (97) 74 (98) 91 (96) 131 (98) 147 (99) 173 (96) 220 (24)		
8	1599	oo	C = 14 Branched fatty acid	132 (100) 147 (98) 117 (97) 91 (95) 74 (54) 220 (26) 205 (8)		
9	1695	oo	Allylphenol + ?	134 (100) 137 (96) 135 (83) 107 (79) 220 (3)		
10	1703	oo	Tetradecanoic acid + Allylphenol	75 (100) 87 (96) 108 (97) 149 (95) 136 (37) 121 (78) 181 (21) 220 (5)		
11	1727	oo	Allylphenol + ?	108 (100) 149 (96) 121 (54) 55 (43) 177 (26)		
12	1738	oo	?	137 (100) 136 (87) 62 (68) 95 (33) 27 (26) 91 (23) 107 (20) 220 (2)		
13	1745	oo	Isopropylphenol	149 (100) 135 (90) 107 (86) 55 (38) 77 (22) 91 (16) 220 (1)	Phenol, isopropyl-	558
14	1883	e	Hexadecanoic acid	74 (100) 149 (98) 55 (94) 87 (63) 236 (1)	13-Octadecanoic acid, methyl ester	385
15	1911	oo	Hexadecanoic acid	74 (100) 89 (100) 56 (98) 143 (40) 227 (12) 270 (6)		
16	1990	e	C ≥ 16 Fatty acid	55 (100) 74 (58) 87 (24) 143 (2)	15-Octadecanoic acid, methyl ester	547
17	2001	e	C ≥ 16 Fatty acid	74 (100) 87 (99) 43 (76) 55 (47) 143 (11)		
18	2064	ooo	Octahydro-2-methylphenanthrene-9-carboxylic acid	148 (100) 197 (99) 121 (98) 117 (87) 91 (76) 257 (22) 272 (14)	Subst. Phenanthrene-9-carboxylic acid	614
19	2088	oo	C ≥ 17 Fatty acid + Isomer of #18	89 (100) 143 (96) 129 (42) 199 (20) 197 (18) 255 (12) 298 (10)		
20	2113	oo	Mixture ?	144 (100) 92 (99) 101 (98) 133 (96) 187 (39) 284 (1) 316 (1)		
21	2137	oo	?	92 (72) 146 (65) 69 (65) 106 (57) 133 (46) 192 (16) 286 (1)		
22	2158	oo	Isomer of 20	144 (100) 91 (64) 55 (58) 122 (39) 284 (1)		
23	2193	oo	?	55 (80) 91 (64) 146 (57) 105 (38) 131 (35) 241 (7) 298 (5)		
24	2210	oo	?	91 (53) 69 (46) 115 (52) 131 (54) 155 (52) 157 (52) 195 (24) 270 (9)		
25	2301	ooo	Mixture ?	145 (100) 215 (66) 241 (63) 211 (58) 157 (40) 171 (47) 299 (2) 314 (1)		

TABLE A-54. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 22E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Ident. Reasonable Elements Match Compound	E.I. No.
1	876	ee	Mixture ?	56 (100) 44 (75) 112 (56) 58 (24) 126 (2)	Piperidine, 1,2,6-trimethyl	519
2	883	ee	Cyanopyridine	104 (100) 78 (74) 51 (34) 77 (28) 103 (51)		
3	918	eee	Alkylantiridine + ?	70 (100) 126 (99) 41 (97) 56 (82) 140 (2)		
4	957	eee	Methylpyridine	93 (100) 86 (99) 65 (60) 63 (18) 32 (18) 41 (16)	Pyridine, 3-methyl	349
5	1006	ee	?	43 (100) 91 (50) 55 (40) 71 (35) 97 (20) 126 (6)		
6	1009	e	?	86 (100) 42 (44) 58 (34) 111 (18) 126 (3)		
7	1199	ee	Alkylantiridine + 1 C ₆ H ₅ gill	72 (100) 44 (56) 128 (10)		
8	1204	ee	Mixture ?	44 (100) 72 (67) 131 (37) 107 (20)		
9	1216	ee	Mixture ?	85 (100) 70 (30) 98 (23) 126 (22) 154 (10) 182 (4)		
10	1303	ee	?	72 (100) 44 (34) 115 (25) 132 (16) 118 (17) 175 (3)		
11	1337	e	?	43 (100) 74 (72) 76 (49) 85 (43) 98 (33) 100 (32) 173 (10)		
12	1353	e	Alkylantiridine	133 (100) 115 (52) 131 (37) 174 (31) 77 (20) 91 (19) 188 (3)		423
13	1374	ee	N,N-dibutyl Formamide	100 (100) 58 (56) 72 (38) 44 (30) 143 (16) 209 (3)	2-Isopropylamine, N-(Phenylmethyl)-	526
14	1393	ee	?	72 (100) 132 (80) 133 (58) 77 (68) 118 (44) 115 (43) 186 (2)	Formamide, N-butyl-N-(1-methyl ethyl)-	
15	1441	ee	?	43 (100) 57 (72) 69 (64) 112 (36) 144 (22) 153 (16) 209 (2)		
16	1461	e	Heptan-3-one, N-(Phenylmethyl)-	132 (100) 105 (63) 86 (50) 77 (28) 146 (26) 188 (31)	2-Isopropylamine, N-(Phenylmethyl)-	638
17	1504	ee	N,N-dibutyl Formamide	100 (100) 58 (52) 72 (37) 143 (25) 94 (26) 214 (3)	Formamide, N-butyl-N-(1-methyl ethyl)-	520
18	1546	ee	?	92 (98) 112 (76) 68 (51) 74 (43) 98 (37) 144 (27) 167 (10)		
19	1811	e	Alkylantiridine	44 (100)		

TABLE A-55. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 23VI

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum
1	.15	--	Air	44 (100)
2	.16	.1-1	Butadiene	54 (100) 33 (80) 35 (48)
3	.18	10-100	Dichloromethane	49 (100) 84, 86 (100) Sat 'd
4	.24	10-100	Chloroform	87 (100) 85 (82) 83 (58) 118 (18) Sat 'd
5	.29	.76	Benzene	78 (100)
6	.35	1-10	Bromodichloromethane	83 (100) 85 (65) 129 (12)
7	.53	.1-1	Toluene	91 (100) 92 (55)
8	.54	.1-1	$\text{C}_2\text{H}_5\text{Cl}$	76 (100) 78 (35)
9	.57	.1-1	Dibromochloromethane	129 (100) 127 (80) 131 (20)
10	.97	.1-1	Ethyl benzene	91 (100) 106 (40)
11	1.00	-(8)	I.S.	
12	1.28	.1-1	C_7 Alkyl benzenes	105 (100) 120 (35)
13	1.50	.1-1	C_8 Alkyl benzene	119 (100) 134 (25)

TABLE A-56. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 23VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13		Air	44(100)
2	0.16	>100	Acetone	43(100)
3	0.17	1-10	Dichloroethylene	61(100)96(40)
4	0.18	10-100	Dichloromethane	49(100)
5	0.24	1-10	Chloroform	83(100)
6	0.24	1-10	Isopropyl ether	45(100)43(43)87(20)
7	0.27	1-10	1,2-Dichloroethane	62(100)64(30)49(30)98,100
8	0.28	10-100	1,1,1-Trichloroethane	97(100)99(70)61(50)117,119,121
9	0.30	10-100	Benzene	78(100)
10	0.45	1-10	C_8H_{16} -- probably 2,4,4-Trimethyl-1-pentene or diisobutylene	57(100)41(50)55(30)97,112
11	0.50	1-10	C_8H_{16} -- probably 2,3,4-Trimethyl-2-pentene	55(100)97(80)41(38)69(30)112(30)
12	0.55	41	Toluene	91(100)
13	0.86	<1	C_7 -Alkyl cyclohexane C_9H_{18}	55(100)97(35)41(35)69(30)126(10)
14	0.88	1-10	C_2 -Alkyl benzene	91(100)106(30)
15	0.91	<1	C_9H_{18} C_3 Alkyl cyclohexane	55(100)41(50)69(40)70(28)91,56,43(18)126(7)
16	0.93	<1	C_3 -Alkyl cyclohexane	55(100)41(34)83(125)69(13)126(8)
17	0.94	<1	C_3 -Alkyl cyclohexane	55(100)83(50)84(30)41(22)69(20)126(6)
18	0.96	<1	C_7 -Alkyl cyclohexane (T)	41(100)69(80)55(68)70(47)104(43)56(38)57(34)111(20)126(12)
19	0.98	<1	C_7 -Alkyl cyclohexane (T)	69(100)55(80)41(68)111(50)56(38)70(27)43(22)126(10)
20	1.00	<1	I.S.	75(100)

TABLE A-57. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 23E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Elements Match	
					Compound	E.L.P. 10 ³
1	1164	ee	Allylformamide	72 (100) 114 (47) 100 (44) 58 (38) 142 (18) 156 (6)	Formamide, N-Butyl-β-(1-Methyl Ethyl)	305
2	1192	ee	Allylamine	72 (100) 106 (34) 86 (28) 44 (24) 55 (22) 142 (19) 156 (4)	Butylamine, N-Methyl-β-(1-Methyl Ethyl)	313
3	1210	ee	Allylformamide	72 (100) 57 (76) 106 (48) 128 (46) 114 (35) 142 (18) 156 (10) 170 (5)	Formamide, N-Butyl-β-(1-Methyl Ethyl)	290
4	1228	eee	Allylformamide	72 (100) 86 (94) 57 (75) 55 (70) 114 (44) 142 (31) 156 (53) 128 (16) 170 (13)		
5	1252	eee	N,N-Allyl-Alkylamide	100 (100) 114 (89) 156 (76) 55 (70) 57 (62) 86 (58) 142 (52) 128 (20) 170 (12)		
6	1311	ee	N,N-Allyl-Alkylamide	142 (100) 86 (82) 70 (68) 55 (58) 37 (52) 100 (60) 156 (66) 170 (14)		
7	1316	ee	N,N-Allyl-Alkylamide	100 (100) 44 (91) 128 (80) 114 (74) 55 (73) 70 (50) 156 (34) 170 (12)		
8	1327	ee	N,N-Allyl-Alkylamide	114 (100) 100 (95) 86 (76) 72 (65) 142 (34) 128 (30) 156 (23) 170 (10)		
9	1331	ee	N,N-Allyl-Alkylamide	128 (100) 100 (96) 37 (48) 70 (47) 170 (7) 184 (3)		
10	1342	ee	N,N-Allyl-Alkylamide	142 (100) 50 (50) 86 (33) 114 (28) 100 (24) 156 (13) 170 (7)		

TABLE A-58. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 24VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.16		Air	44 (100)
2	0.21	1-10	Dichloroethylene	61 (100) 96 (80) 98 (50)
3	0.21	<10	Dichloroethane	49 (100)
4	0.27	<10	Chloroform	83 (100)
5	0.31	1-10	1,1,1-Trichloroethane	97 (100) 99 (70) 61 (45) 117, 119, 121
6	1.00	~ (8)	I.S.	75 (100)

TABLE A-59. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 25VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13		Air	44(100)
2	0.14	1-10	Butene or Methyl (C_4H_8) propane	41(100) 56(55)
3	0.17	10-100	Acetone	43(100)
4	0.17	1-10	C_3H_{10} + Unknown	41(100) 59(80) 40(40) 55(25) 63(15) 70(12) 78(5)
5	0.18	1-10	Ethanol	62(100) 47(85) 45(52) 46(30) 61(30) 63(64) 64(4)
6	0.18	1-10	Dichloromethane	49(100)
7	0.21	1-10	S-containing Unknown	110(100) 95(95) 93(90) 108(50) 112(20)
8	0.24	10-100	Methylethyl sulfide	61(100) 76(55) 48(52)
9	0.27	1-10	1,2-Dichloroethane	62(100) 56(40) 64(35) 69(20) 98(100) 3
10	0.28	<1	1,1,1-Trichloroethane	97(100) 61(70) 99(60) 117(119) 121
11	0.31	1-10	2-Pentanone	43(100) 86(15) 71(4)
12	0.38	1-10	Diethyl sulfide	75(100) 47(90) 90(70) 81(62) 60
13	0.41	1-10	Methyl n-propyl sulfide	61(100) 90(50)
14	0.46	10-100	Dimethyl Disulfide	94(100) 45(72) 79(65)
15	0.57	1-10	3-Methyl-2-thiaphene	75(100) 41(80) 106(60) 56(45)
16	0.62	1-10	Thiacyclopentane	60(100) 88(60) 41(38)
17	0.65	1-10	Unknown Mixture	142(100) 45(95) 127(65) 94(37) 140(47) 47(61) 37
18	0.75	1-10	M 108 S-unknown	80(100) 108(99) 45(50) 84(40)
19	0.79	1-10	2-Methyl tetrahydrothiophene	87(100) 102(40)
20	0.87	1-10	3-Methyl thiacyclopentane	60(100) 102(90) 41(68) 45(67) 74(40) 87(50)
21	0.91	1-10	Methyl thiacyclopentane	101(100) 67(70) 87(65) 41(65) 116(40)
22	0.94	1-10	Dimethyl thiacyclopentane	101(100) 59(52) 67(40) 116(45)
23	0.95	1-10	Dimethyl thiacyclopentane	101(100) 59(50) 116(50)
24	0.97	10-100	2,3-Dithiaphene	80(100) 122(45)
25	0.99	1-10	Unknown	156(100) 128(95) 134(126) 50
26	0.99	<1	Methylthiacyclopentane	101(100) 116(60) $\text{C}_6\text{H}_{12}\text{S}$ M116
27	1.00	~(8)	1.5.	75(100)
28	1.01	<1	$\text{C}_6\text{H}_{12}\text{S}$	101(100) 116(50) 41(50) 59(40)
29	1.02	<1	$\text{C}_6\text{H}_{12}\text{S}$	101(100) 116(50) 59(50) 41(48)
30	1.06	10-100	$\text{C}_6\text{H}_{10}\text{S}_2$ (3,4-Dithiaphene)	86(100) 122(90) 94(40)

TABLE A-59. (Continued)

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
31	1.06	1-10	Methylthiacyclobenzene	101(100) 118(70) 67(50) 87(40) $C_6H_7S^+$
32	1.08	1-10	Unknown	41(100) 43(90) 80(75) 45(60) 47(28) 46(25) 84(20) 74(10) 116(6) 130(3)
33	1.13	1-10	Unknown	87(100) 116(20) 130(5)
34	1.16	1-10	Unknown	128(100) 43(78) 41(65) 136(50) 170(30) 130(21) 124, 125(20) 112, 148(18)
35	1.17	1-10	Unknown	115(100) 81(60) 101, 130(50) 59, 60, 81(33) 75(28)
36	1.21	10-100	S-containing Unknown	94(100) 66(60) 43(55) 136(46) 41(29) 59(15)
37	1.23	1-10	Unknown	101(100) 59(33) 67(30) 130(10)
38	1.23	1-10	Unknown	101(100) 130(30) 59(30) 67(28)
39	1.30	10-100	S-containing Unknown	94(100) 136(70) 43(65) 66(55) 61(42)
40	1.32	10-100	Dimethyl dithiobenzene	43(100) 108(30) 61(28) 150(10)
41	1.41	1-10	Dimethyl dithiobenzene	63(100) 108(30) 61(25) 150(12)
42	1.43	1-10	S-containing Unknown	94(100) 41(40) 57(33) 66(30) 150(13)
43	1.62	1-10	3-Methyl-1-(1-thiethylbenzene) + H ₂ O	138(100) 91(90) 45(72) 73(60) 153(50) 148(10)
			Unknown	

TABLE A-60. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 25E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Structure	Ref. No.
1	852	00	8-containing ?	80(100) 106(81) 45(37) 64(48) 110(7)		
2	868	00	Ethylbenzene	91(100) 106(38) 105(21) 77(21) 51(23)	Benzene, 1,2-Dimethyl	549
3	880	00	2,3-Dichlorobenzene	80(100) 45(51) 45(38) 122(37) 64(26)		
4	884	00	Xylene	91(100) 106(36) 51(22) 77(18) 65(12) 63(11)	Benzene, Ethyl	407
5	903	00	3,4-Dichlorobenzene	66(100) 122(69) 96(52) 79(11)		
6	952	00	Methyldichlorobenzene ($\text{C}_6\text{H}_4\text{Cl}_2$)	94(100) 45(80) 66(45) 136(40) 59(27)		
7	1035	00	?	Four Spectra		
8	1042	00	?	67(100) 55(69)		
9	1047	00	$\text{C} \geq 11$ - Alkene	55(100) 85(78) 98(15)	2-Pentene, 4,4-Dimethyl	586
10	1154	00	Benztolene + ?	85(100) 128(83) 119(64) 91(46) 59(64) 48(40) 100(49)		
11	1235	00	C_5 -Alkylbenzene	133(100) 63(70) 79(64) 77(56) 105(46) 31(32) 91(23)	Benzene (1-Methyl Butyl)	323
12	1249	00	10-Inden-1-one, Dihydro	104(100) 132(78) 78(62) 51(38) 77(39) 76(20) 133(9)	10-Inden-1-one, 2,3-Dihydro	672
13	1263	0	3(20)-Benzofuranone, Methyl	91(100) 119(83) 148(79) 63(64) 77(29)	3(20)-Benzofuranone, 7-Methyl	555
14	1282	00	C_5 -Alkylbenzene	133(100) 105(62) 77(64) 148(30) 91(25) 103(21) 119(20)	Benzene, 1-Ethyl-3-(1-Methyl Ethyl)	547
15	1307	00	3(20) Benzofuranone, Methyl	119(100) 148(86) 91(70) 89(61) 63(56) 77(41) 132(41)	3(20) - Benzofuranone, 7-Methyl	476
16	1324	00	C_5 -Alkylbenzene	118(100) 117(84) 91(40) 63(60) 77(37) 146(32)		
17	1347	00	Ethanone, 1-(4-(1-Methylethyl) Phenyl)-	147(100) 91(75) 63(64) 119(63) 162(68) 78(37) 105(12)	Ethanone, 1-(4-(1-Methylethyl) Phenyl)-	528
18	1361	00	10-Indene, 1-Ethyl-2,3-Dihydro	117(100) 146(70) 118(52) 115(40) 91(36) 63(33) 51(28) 89(23) 103(16)	10-Indene, 1-Ethyl-2,3-Dihydro	467
19	1385	00	Alkyl-Alcohol $\text{C} \geq 11$	69(100) 84(86) 70(56) 55(46) 97(6) 91(4)		
20	1400	00	Heptadecane + ?	57(100) 70(72) 69(68) 111(53) 95(23) 85(17) 77(13)		
21	1482	00	$\text{C} \geq 16$ Alkane	57(100) 71(57) 85(34) 99(8) 115(6) 97(6) 149(6)	Tridecane, 2-Methyl	506
22	1700	00	Heptadecane + ?	57(100) 71(82) 85(34) 91(23) 128(21) 148(20) 165(27)		
23	1723	00	C_2 -1,1'-Biphenyl	153(100) 152(75) 154(73) 182(92) 181(21) 151(25) 76(39) 63(36)		
24	1742	00	C_2 -1,1'-Biphenyl	153(100) 152(62) 154(65) 151(28) 182(75) 183(18)	[1,1'-Biphenyl]-4-Carbaldehyde	403
25	1800	00	Octadecane	57(100) 63(89) 71(67) 85(44) 99(12) 165(6)	Heptadecane, 2-Methyl	539
26	1907	00	Nonadecane	57(100) 63(94) 71(62) 85(38) 99(10)	Pentacosane	644

TABLE A-61. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 26VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum
1	--	--	Air	44(100)
2	0.18	>>>100	Dichloromethane	49(100)
3	0.19	>100	$\text{C}_6\text{H}_5\text{Cl}$ (?)	86(100) 51(65) 48(40) 47(35) 88(15) 83(10)
4	--	>100	$\text{C}_6\text{H}_5\text{Cl}$ (?)	47(100) 51(93) 86(70) 48(55) 88(20) 83(20)
5	0.30	1-10	Benzene	78(100)
6	0.48	>100	Probably C_6H_6 , e.g., Tetramethyl cyclopropane	55(100) 83(70) 41(55) 42(40) 98(30)
7	0.49	>100	Dimethyl disulfide (2,3-dithiabutane)	94(100) 45(70) 79(60) 41(35) 35(35)
8	0.50	>100	C_6 ketone + C_6H_{12}	43(100) 49(25) 58(15) 84(15) 57(12) 85, 86(8) 41, 100(5)
9	0.53	10-100	C_6H_6 , e.g., Trimethyl cyclopentane	70(100) 55(90) 41(38) 97, 112(6)
10	0.55	>>100	Toluene	91(100)
11	0.60	10-100	2,3-Dimethylhexane	43(100) 70(45) 71(30) 41(25)
12	0.60	10-100	Alkane	57(100) 43(98) 71(12) 99(9) 114(2)
13	0.62	10-100	Alkane	43(100) 57(60) 41(40) 55(22) 70(10) 97(9) 71, 9(5)
14	0.64	10-100	C_6H_6 Methyl cycloheptane	55(100) 97(60) 112(20)
15	0.64	10-100	C_6H_6 , e.g., Dimethylhexane	43(100) 57(50) 41, 85(25)
16	0.67	10-100	Hydrocarbon	55(100) 83(60) 56(40) 42, 41(58)
17	0.68	10-100	Alkane M112	55(100) 41(58) 56(55) 83(67) 70(40) 42(35) 69(30) 97, 112(12)
18	0.70	10-100	Alkane M112	55(100) 97(65) 41(40) 56(33) 42(32) 69(27) 112(20) 70(18)
19	0.73	10-100	Hydrocarbon	43(100) 41(40) 57(30) 85(22) 55, 56(20) 42(18) 71(15) 97(5) 114(3)
20	0.75	>100	Alkane	43(100) 41(35) 57(28) 85(22) 71(15) 114(2)
21	0.85	>100	Hydrocarbon	55(100) 83(90) 41(72) 43, 42(42) 56(22) 42(20) 67, 69, 112(18)
22	0.88	>100	Hydrocarbon	43(100) 41(45) 57(40) 42, 49, 71(25) 111(122) 96, 55(70) 85(100) See 113, 1-128
23	0.90	>100	Hydrocarbon + C_2 alkyl benzene	57(100) 43(55) 41(50) 91(45) 55(40) 56(28) 71(18) 70(15)
24	0.91	>100	C_2 Alkyl benzene	91(100) 106(25)
25	0.93	>100	C_2 Alkyl benzene	91(100) 106(30)
26	0.97	>100	C_2 Alkyl benzene	91(100) 106(38)
27	1.00	>100	Hydrocarbon	43(100) 41(35) 57(22) 71(16) 55, 85(13) 70(12)
28	1.01	>100	Hydrocarbon	41(100) 57(70) 82, 49(55) 56(52) 43, 55(48) 111(23) 40(18) 126(8)
29	1.05	100	C_2 Alkyl benzene	91(100)

TABLE A-61. (Continued)

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
30	1.05	>100	Hydrocarbon	57(100)41(20)83(10)75(5)110(2)
31	1.06	>100	Hydrocarbon	55(100)97(50)41(45)69(26)56(23)126(5)
32	1.12	>100	C ₉ Alkane	43(100)57(65)41(40)42, 56, 85(18)40, 71, 55(10)99(2)128(1)
33	1.14	>100	C ₃ -Alkyl benzene	105(100)120(20)
34	1.22	>100	C ₃ -Alkyl benzene	91(100)120(20)
35	1.25	>100	C ₃ -Alkyl benzene	105(100)120(20)
36	1.28	>100	C ₃ -Alkyl benzene	120(100)105(80)
37	1.30	>100	C ₃ -Alkyl benzene	105(100)
38	1.35	>100	Unknown	120(100)119(30)
39	1.37	10-100	C ₄ -Alkyl benzene	105(100)77, 79(15)134(1)
40	1.40	>100	C ₃ -Alkyl benzene	105(100)120(30)
41	1.41	>100	C ₄ -Alkyl benzene	119(100)91(30)134(15)
42	1.42	>100	C ₉ H ₁₀ , e.g., Methyl styrene	117(100)118(50)115(30)
43	1.44	10-100	Substituted cyclohexane	55(100)83(78)43(75)71(62)82(55)
44	1.47	>100	C ₄ -Alkyl benzene	105(100)119(45)134(20)
45	1.50	>100	Unknown	105(100)77(15)
46	1.56	>100	Unknown hydrocarbon	55(100)97(62)41(24)96(12)111(5)
47	1.57	>100	C ₄ + C ₅ -Alkyl benzene	119(100)105(80)91(40)134(20)133(13)148(8)
48	1.60	>100	Alkane	43(100)57(90)71(35)85(20)
49	1.63	>100	C ₁₀ H ₁₂ (ethyl styrene)	117(100)115, 132(23)
50	1.65	10-100	C ₅ -Alkyl benzene	105(100)148(2)
51	1.67	10-100	C ₅ -Alkyl benzene	119(100)91, 133, 148(13)
52	1.69	10-100	Naphthalene	128(100)

TABLE A-62. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 26E

GC Peak No.	Retention Time, min	Amount, µg/l	Tentative Identification	Characteristic Ion in Mass Spectrum	Most Reasonable Monomer Methyl	E.I. No.
1	871	+++	Butylacetate	43(100)51(30)44(15)73(16)61(16)	Acetic Acid, Butyl Ester	485
2	883	++	Ethylbenzene	91(100)105(25)77(13)65(12)51(12)	Benzene, Ethyl	520
3	888	++	Xylene	91(100)106(37)77(15)51(16)65(11)	Benzene, Ethyl	613
4	900	+++	Xylene	91(100)106(37)105(15)77(14)51(13)65(12)	Benzene, 1,4-Dimethyl	470
5	904	++	2-Methoxyphenol	57(100)45(48)41(43)87(18)75(9)	Ethanol, 2-Methoxy	802
6	938	++	C ₃ -Alkylbenzene	91(100)65(21)120(18)51(15)77(10)	Benzene, propyl-	603
7	946	++	C ₃ -Alkylbenzene	105(100)120(26)77(21)91(18)51(13)65(11)	Benzene, 1-Ethyl-2-Methyl	636
8	955	++	C ₃ -Alkylbenzene	105(100)120(26)77(21)91(18)51(13)65(11)	Benzene, 1-Ethyl-2-Methyl	593
9	965	++	C ₃ -Alkylbenzene	105(100)120(25)77(20)79(18)91(18)51(15)	Benzene, 1-Ethyl-2-Methyl	617
10	981	+++	C ₃ -Alkylbenzene	105(100)120(25)77(18)91(13)51(11)65(8)	Benzene, 1-Ethyl-2-Methyl	678
11	1003	++	Decane	57(100)65(99)51(70)71(38)85(30)	Hexane 3,3-Dimethyl	575
12	1006	+++	C ₃ -Alkylbenzene	105(100)120(35)77(15)91(12)51(10)65(7)	Benzene, 1-Ethyl-2-Methyl	633
13	1016	++	Methylstyrene	117(100)116(60)115(34)91(25)63(18)51(12)	Benzene, 1-Ethyl-3-Methyl	550
14	1021	++	Ethylbenzene	57(100)41(35)35(38)70(21)83(18)117(12)	1-Hexanol, 2-Ethyl-	610
15	1035	+++	C ₄ -Alkylbenzene	105(100)119(92)91(38)136(37)77(26)51(15)	Benzene, 1,2-Diethyl	695
16	1041	+++	C ₄ -Alkylbenzene	105(100)134(24)77(19)91(15)51(10)119(11)	Benzene (1-Methylpropyl)	637
17	1045	+++	C ₄ -Alkylbenzene	105(100)119(64)91(50)134(32)77(25)51(15)65(12)	Benzene, 1,2-Diethyl	743
18	1051	++	C ₄ -Alkylbenzene	119(100)134(24)91(20)77(18)51(11)	Benzene, 2-Ethyl-1,4-Dimethyl	623
19	1055	++	C ₄ -Alkylbenzene	105(100)134(18)77(19)91(12)51(11)	Benzene (1-Methylpropyl)-	511
20	1062	+++	C ₄ -Alkylbenzene	119(100)91(30)134(29)77(17)51(10)65(9)	Benzene, 2-Ethyl-1,4-Dimethyl	636
21	1068	+++	C ₄ -Alkylbenzene	119(100)91(26)134(24)77(13)41(12)57(11)105(11)	Benzene, 2-Ethyl-1,4-Dimethyl	606
22	1087	+++	C ₅ -Alkylbenzene	119(100)91(34)134(24)105(21)77(18)51(12)65(11)145(4)	Benzene, (1,1-Dimethylpropyl)	470
23	1104	+++	HC + C ₅ -Alkylbenzene	57(100)45(95)71(64)85(21)119(25)134(12)140(1)	Benzene, 1,2,3,5-Tetramethyl	542
24	1118	+++	C ₆ -Alkylbenzene	119(100)134(30)91(22)77(12)65(7)	Benzene, 1,2,4,5-Tetramethyl	671
25	1127	+++	Ethylstyrene + HC	117(100)132(33)91(23)77(13)63(11)148(3)	Benzene, 1-Ethyl-4-Ethyl	502
26	1133	+++	C ₅ -Alkylbenzene	117(100)119(55)91(34)115(35)132(30)148(11)	Benzene (1-Ethylpropyl)	447
27	1136	++	C ₆ -Alkylbenzene	119(100)134(34)91(25)77(14)51(11)	Benzene (1,2,3,5-Tetramethyl)	646
28	1157	+++	Naphthalene	128(100)73(19)51(13)63(11)102(15)119(13)148(2)	Naphthalene	258
29	1164	++	C ₅ -Alkylbenzene	131(100)148(25)91(22)105(17)77(15)51(11)	Benzene, 1-Ethyl-2,4,5-Trimethyl-	580
30	1193	++	C ₅ -Alkylbenzene	131(100)134(73)91(30)105(21)77(18)51(12)	Benzene, 1-Ethyl-1,4-Dimethyl	576

TABLE A-62. (Continued)

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Numerous Ions in Mass Spectrum	
					Compound	$\frac{M}{m}$, 10 ³
31	1203	oo	Decane	57(100)43(89)41(65)71(54)85(28)98(5)99(5)	Decane	767
32	1244	oo	Methylisophtalene	142(100)141(88)115(60)93(23)63(20)143(10)	Naphthalene, 2-methyl	272
33	1335	ooo	C $\geq$ 13 Alkane	71(100)43(92)41(63)56(35)55(33)83(26)173(3)	1-Hexene, 3,4,5-Trimethyl	356
34	1355	ooo	Alkyl-Alcohol C $\geq$ 12	71(100)43(93)56(76)89(55)154(13)172(6)	1-Butanol, 4-(Mesityl)-	502
35	1515	oo	Trichloro - 7	247(100)245(78)203(30)202(40)249(48)251(10)		
36	1943	oo	Trichloro - 7	118(100)47(69)63(6)764(43)262(32)267(20)279(33)277(26)281(17)		
37	1946	oo	C $\geq$ 19 Alkane	57(100)43(95)71(66)85(41)127(5)		663
38	1999	ooo	Trichloro - 7	79(100)118(60)63(46)245(20)293(15)297(10)299(12)	Tetradecane	
39	2101	oo	Nonacosane	57(100)43(89)71(65)85(41)99(12)113(7)155(2)	Pentacosane	766
40	2202	oo	Docosane	57(100)43(88)71(67)85(44)99(14)113(8)127(6)141(4)	Pentacosane	813
41	2306	oo	Tricosane	57(100)43(85)71(68)85(44)99(14)113(9)127(6)	Tetradecane	770
42	2291	oo	Butylbenzyl-Phthalate	149(100)91(90)65(27)104(20)123(12)206(11)	1,2-Hemmedicarboxylic Acid, Butyl 2-Methylpropyl Ester	349
43	2405	oo	Tetradecane	57(100)43(82)71(69)85(47)99(18)113(11)155(4)	Tetradecane	733
44	2509	oo	Pentacosane	57(100)43(82)71(68)85(45)99(15)113(10)127(6)141(5)183(1)	Pentacosane	728
45	2551	oo	C $\geq$ 23 Alkane	57(100)43(82)71(67)85(44)113(10)183(1)	Docosane, 11-Decyl-	796
46	2605	oo	Hexacosane	57(100)43(78)71(68)85(46)99(16)113(10)183(2)	Docosane, 11-Decyl-	707
47	2696	oo	Heptacosane	57(100)43(80)71(67)85(44)99(16)113(10)127(7)	Tetradecane	643
48	2803	oo	Octacosane	57(100)43(84)71(66)99(14)113(9)155(2)	Tetradecane 3,5,24-Trimethyl	687
49	2905	oo	Nonacosane	57(100)43(83)71(61)85(40)99(15)113(10)127(6)	Tetradecane 3,5,24-Trimethyl	571

TABLE A-63. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 26E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum	Mass Spectrometric Molecular Weight	
					Compound	M^+
1	895	00	2-Necety ethanol	57(100)43(83)41(68)87(26)75(12)100(2)	Ethanol, 2-Necety	790
2	906	00	Hexanoic acid	74(100)43(99)59(61)87(56)55(39)99(26)101(11)	Hexanoic acid, methyl ester	323
3	1004	00	Heptanoic acid	74(100)43(64)87(30)59(18)101(10)113(9)	Heptanoic acid, methyl ester	452
4	1027	000	C $\geq$ 8 Fatty acid	57(100)87(99)102(99)59(63)69(23)115(20)130(16)	Hexanoic acid, 2-ethyl, methyl ester	627
5	1041	00	Hexanoic acid	105(100)77(66)136(23)51(20)119(18)	Hexanoic acid, methyl ester	517
6	1103	00	Octanoic acid	74(100)43(53)87(40)55(28)57(23)59(22)127(5)	Octanoic acid, methyl ester	636
7	1146	00	Methylhexanoic acid	91(100)119(96)118(69)65(40)90(28)150(28)	Hexanoic acid, 2-methyl, methyl ester	603
8	1203	00	Nonanoic acid	74(100)87(59)63(46)55(28)59(19)141(6)143(5)	Nonanoic acid, methyl ester	691
9	1274	00	Decanoic acid	74(100)87(48)63(46)55(18)59(12)143(8)155(4)157(1)	Decanoic acid, methyl ester	756
10	1340	00	Trimethylhexanoic acid	146(100)147(77)119(79)91(70)131(60)77(48)103(42)178(33)	Hexanoic acid, 2,4,5-Trimethyl methyl ester	526
11	1355	00	Trimethylhexanoic acid	147(100)91(67)119(42)77(26)178(26)	Hexanoic acid, 2,4,5-Trimethyl, methyl ester	722
12	1391	00	?	103(100)43(67)71(63)74(60)61(26)163(2)		
13	1505	0	Dodecanoic acid	74(100)87(36)163(8)171(3)214(1)	Dodecanoic acid, methyl ester	716
14	1517	000	Trichloro + ?	247(100)245(80)249(47)251(10)		
15	1672	00	Nonanesulfonamide H,4-Dimethyl	91(100)45(28)135(12)185(7)121(6)	Nonanesulfonamide, H,4-Dimethyl	616
16	1706	00	Tetradecanoic acid	74(100)87(55)163(8)199(2)	Tetradecanoic acid, methyl ester	810
17	1911	00	Hexadecanoic acid	87(100)74(99)43(90)55(61)143(17)270(2)	Hexadecanoic acid, methyl ester	549
18	1980	00	C $\geq$ 14 Fatty acid	74(100)87(62)143(12)199(2)241(2)	Cyclopentamethyldecanoic acid, methyl ester	646
19	2007	0	C $\geq$ 15 Fatty acid	74(100)87(60)143(8)199(2)	Nonacosanoic acid, methyl ester	649
20	2049	00	C $\geq$ 17 Fatty acid	67(100)81(73)41(58)55(47)95(32)109(25)	9,12,15-Octadecatrienoic acid, methyl ester (6,8,9)	691
21	2073	000	Octadecadienoic acid	67(100)81(75)55(69)41(66)95(45)109(18)197(4)	12,15-Octadecadienoic acid, methyl ester	680
22	2085	000	Octadecanoic acid	55(100)69(86)74(79)87(47)143(2)264(3)	10-Octadecanoic acid, methyl ester	743
23	2113	00	Octadecanoic acid	87(100)74(99)43(74)55(49)143(17)199(4)298(1)	Heptadecanoic acid, 15-methyl, methyl ester	695
24	2120	00	Octadecadienoic acid	67(100)81(70)95(30)299(3)	12,15-Octadecadienoic acid, methyl ester	734
25	2163	00	Octadecadienoic acid	67(100)81(66)41(67)55(44)95(38)109(15)294(0.5)	12,15-Octadecadienoic acid, methyl ester	977
26	2249	00	C $\geq$ 18 Fatty acid	67(100)81(73)41(88)55(88)	9,12,15-Octadecatrienoic acid, methyl ester	687
27	2298	00	C $\geq$ 18 Fatty acid	55(100)87(70)74(45)	Octadecanoic acid, 12-hydroxy, methyl ester	676

TABLE A-64. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 27VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.10	--	Air	44(100)
2	0.14	>100	Acetone	43(100) 58(70)
3	0.21	>>>100	Isopropyl alcohol	45(100) 43(20) 59(2)
4	1.00	-(8)	I.S.	75(100)

TABLE A-65. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 28VE

GC Peak No.	Relative Retention Time	Amount, μ g/l	Typical Identification	Characteristic Ions in Mass Spectrum
1	.14		Air	44(100)
2	.15	10-100	Butene tetracetaldehyde (T)	44(100)43(58)41(48)56(32)42(22)
3	.17	>100	Acetone	43(100)
4	.19	>100	Dichloromethane	49(100)
5	.20	>100	Isobutyraldehyde	43(100)41(60)72(40)
6	.21	1-10	2-Methylpropenal (methacrolein)	41(100)70(70)42(30)41(25)
7	.23	10-100	Methyl ethyl ketone	43(100)72(18)
8	.25	1-10	Chloroform + C ₂ Hydrocarbon	41(100)43(96)57(95)82(90)85(60)
9	.30	1-10	1,1,1-Trichloroethane	97(100)81(70)99(60)117,119,121
10	.34	1-10	Tetramethylcyclopropane (T)	55(100)83(60)41(40)98(20)
11	.49	1-10	n-Heptane	43(100)37(28)85(10)100(5)
12	.56	>100	Toluene	91(100)92(60)
13	.62	10-100	Ethyl methyl-1,3-dioxolane	87(100)59(90)41(50)72(20)110(5)
14	.89	>100	Unknown	106(100)65(60)51(50)
15	.66	>100	C ₂ Ketone	43(100)71(20)87(5)114(5)
16	.86	1-10	Unknown	87(100)59(80)41(60)56,43(38)129(2)
17	.87	>100	C ₂ Alkyl benzene	91(100)106(30)
18	.97	>100	Cyclooctatetraene	104(100)78(60)51(32)
19	.98	>100	C ₂ Alkyl benzene	91(100)106(50)
20	1.05	1-10	Unknown	43(100)71(75)41(52)56(40)89(12)101(2)
21	1.05	1-10	C ₃ Alkyl benzene	105(100)120(20)
22	1.12	1-10	C ₃ Alkyl benzene	91(100)120(20)
23	1.15	10-100	C ₃ Alkyl benzene	105(100)120(20)
24	1.15	10-100	C ₃ Alkyl benzene	105(100)120(22)
25	1.17	10-100	C ₃ Alkyl benzene	105(100)120(35)
26	1.18	10-100	C ₁₀ Methyl styrene	118(100)117(95)103(60)78(50)
27	1.20	>100	Unknown	55(100)89(95)115(90)41(60)45(46)43(42)71(20)157(3)
28	1.22	10-100	C ₃ Alkyl benzene	105(100)120(38)
29	1.25	>100	Hydrocarbon	57(100)56(73)41(65)72(40)
30	1.28	10-100	C ₃ Alkyl benzene	105(100)120(35)

TABLE A-65. (Continued)

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Testione Identification	Characteristic Ions in Mass Spectrum
31	1.30	1-10	$\text{C}_{10}\text{H}_{18}\text{O}$ Methyl styrene	117(100)118(40)115(30)65(18)91(17)
32	1.33	10-100	C_6 Alkyl benzene	105(100)119(75)134(25)
33	1.34	1-10	C_6 Alkyl benzene	105(100)134(12)
34	1.35	10-100	C_6 Alkyl benzene	105(100)119(50)91(40)134(28)
35	1.35	10-100	C_6 Alkyl benzene	119(100)91(30)134(18)
36	1.37	1-10	C_6 Alkyl benzene	105(100)134(5)
37	1.39	10-100	C_6 Alkyl benzene	119(100)91(28)134(20)
38	1.39	10-100	C_6 Alkyl benzene	119(100)134(15)
39	1.41	10-100	C_6 Alkyl benzene	119(100)91(30)134(20)
40	1.41	1-10	C_6 Alkyl benzene + alkane	119(100)134(20)
41	1.44	1-10	C_6 + C_7 Alkyl benzene	119(100)105(67)91(40)134(12)148(13)
42	1.46	1-10	C_6 Alkyl benzene	119(100)134(20)
43	1.47	10-100	C_6 Alkyl benzene	119(100)134(20)91(22)
44	1.49	1-10	C_7 -Styrene	117(100)115(30)132(25)
45	1.50	1-10	C_7 Alkyl benzene	119(100)91(29)148(12)
46	1.51	1-10	C_7 Alkyl styrene + C_7 Alkyl benzene	117(100)115(27)132,133(20)148(5)
47	1.52	1-10	C_7 Alkyl benzene	119(100)91(30)148(9)
48	1.52	1-10	C_6 Alkyl benzene	119(100)134(30)
49	1.52	1-10	Unknown	105(100)106(82)104(75)91(60)132,148(12)
50	1.56	1-10	Naphthalene	128(100)
51	1.61	1-10	C_7 Alkyl benzene	133(100)105(30)91(29)148(20)
52	1.64	1-10	Alkene	43(100)57(95)71(45)85(20)
53	1.92	>100	Biphenyl	154(100)151(50)77(38)
54	1.97	>100	Diphenyl ether	51(100)77(93)170(90)141(70)142(65)115(60)

TABLE A-66. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 28E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Benzene Match	
					Compound	R.I. $\times 10^3$
1	853	++	Dimethyl-3-Pentenoate	43(100)71(90)41(42)70(20)116(16)87(3)	3-Pentenoate, 2,4-Dimethyl	516
2	866	+++	Ethylbenzene	91(100)106(25)31(13)65(11)77(8)	Benzene, Ethyl-	769
3	878	+++	O-Xylene	91(100)106(68)31(31)65(26)77(26)	Benzene, 1,4-Dimethyl	536
4	890	+++	P-Xylene	91(100)106(88)77(30)105(38)51(36)	Benzene, 1,4-Dimethyl	429
5	903	++	2-Autoxyethanol	57(100)45(50)41(44)46(25)87(18)75(10)		
6	928	++	Propanoic Acid, 2-Methylpropyl Ester	71(100)43(81)46(57)57(51)89(23)91(8)106(3)	Propanoic Acid, 2-Methylpropyl Ester	581
7	942	++	C ₃ -Alkylbenzene + ?	56(100)41(60)105(57)69(51)57(43)115(33)120(12)		
8	964	+++	Mixture ?	56(100)69(94)115(86)71(26)73(12)157(4)		
9	974	++	C ₃ -Alkylbenzene	105(100)120(33)77(20)91(15)51(15)121(2)	Benzene, 1,2,4-Trimethyl-	664
10	1002	++	Decane			
11	1099	++	Undecane			
12	1355	+++	1,1'-Biphenyl	154(100)153(61)152(31)76(25)51(17)63(13)	1,1'-Biphenyl	580
13	1389	+++	Diphenyl Ether	51(100)77(97)141(49)170(50)	Benzene, 1,1'-Oxybis-	461

TABLE A-67. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 28E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Benzene Match	
					Compound	R.I. $\times 10^3$
1	907	++	C ₂ & 6 Fatty acid	74(100)42(58)59(34)87(33)79(16)101(8)	Pentanoic acid, 3-methyl, methyl ester	560
2	987	++	Geritol	45(100)59(43)72(23)43(22)89(2)103(2)106(1,7)	Ethanoic acid, 1,1'-Oxybis[2-ethoxy-	595
3	999	+++	Phenol	94(100)66(71)40(21)95(7)	Phenol	557
4	1063	++	Benzoic acid	105(100)77(47)51(61)136(28)106(8)	Benzoic acid, methyl ester	603
5	1105	++	Octanoic acid	74(100)41(61)55(32)87(40)127(7)	Octanoic acid, methyl ester	670
6	1363	++	Diphenyl ether	170(100)141(89)31(83)77(64)115(36)169(25)	Benzene, 1,1'-Oxybis-	597
7	1506	++	Dodecanoic acid	74(100)41(56)67(56)55(38)115(8)170(7)183(1)	Cyclopentadecanoic acid, methyl ester	489
8	2070	++	Octadecanoic acid	67(100)41(90)55(80)81(69)95(40)109(16)197(6)	9,11-Octadecanoic acid, methyl ester	609
9	2080	++	Octadecanoic acid	41(100)55(99)53(69)50(74)46(87)265(100)(2)	10-Undecanoic acid, methyl ester	516
10	2165	++	C ₂ & 18 Fatty acid	74(100)87(70)43(50)41(38)55(34)145(16)199(4)	Heptadecanoic acid, methyl ester	859
11	2298	++	C ₃ -Alkyl, octahydro, phenanthrene carbonylic acid	43(100)141(65)55(61)59(59)239(80)299(10)314(4)	1-Phenanthrene carbonylic acid, ethyl-7-(1-methyl ethyl)-methyl ester	445

TABLE A-68. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 29VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	--	Air	44(100)
2	0.18	1-10	Dimethyl sulfide (8)	62(100)47(82)45(68)46(35)61(70)74(102)109,110(2)
3	0.18	1-10	Dichloromethane	49(100)
4	0.20	<1	1,1-Dichloroethane + Ethyl isopropyl ether (7)	45(100)43(80)43(70)65(28)98(6)100(3)
5	0.23	1-10	Hexane (7)	56(100)41(80)55(70)
6	0.24	1-10	Chloroform	83(100)
7	0.27	10-100	Dichloroethane	62(100)44(75)49(72)
8	0.29		Dichloroethane	49(100)44(100)42(83)43(45)98,100
9	0.31	1-10	Hexane	78(100)
10	0.48	<1	Dimethyl disulfide	94(100)46(70)79(60)46(38)
11	0.53	<1	1,1,2-Trichloroethane (8)	97(100)83(92)41(70)99(40)85(60)132,134(5)136(3)
12	0.55	1-10	Toluene	91(100)92(50)
13	0.62	1-10	1,1-Dichloroethane	107(100)109(90)
14	0.69	10-100	Octene	43(100)55(78)70(40)83(20)112(4)
15	0.72	<1	Octene	43(100)41(40)56(30)85(25)71(15) 5m 114
16	0.74	<1	2-Octene M 112	55(100)41(70)70(30)112(30)
17	0.76	<1	S-containing unknown	80(100)108(95)45(45)44(40)
18	0.77	<1	$\text{C}_{10}\text{H}_{18}$ (octene or trimethyl cyclopentane)	55(100)41(80)56(60)70(45)112(30)
19	0.98	1-10	Dimethyl hexene (7)	55(100)41(28)49(22)83(20)126(12)97(10)
20	1.00	- 8	15	75(100)
21	1.05	1-10	Ethyl-1-methyl ethyl disulfide $\text{C}_8\text{H}_{18}\text{S}_2$	66(100)122(60)94(55)
22	1.06	<1	Nonane M128	43(100)55(85)85(30)
23	1.24	<1	$\text{C}_{10}\text{H}_{20}$ eg Methyl nonane	55(100)56(65)49(58)47(50)41(45)58(30)70(20)83(18)140(3)
24	1.25	<1	Unknown	41(100)43(58)48(50)
25	1.27	1-10	$\text{C}_{10}\text{H}_{18}$ eg 5-Methyl-4-hexene	55(100)49(70)56(50)41(40)83(20)70(19)140(8)
26	1.29	10-100	1-Decene	56(100)55(92)41(85)43(70)65(65)55(55)57(54)83(30)
27	1.30	1-10	$\text{C}_{10}\text{H}_{20}$ eg Dimethyl octene	43(100)55(85)41(84)58(72)56(62)70(45)71(42)71(12)111(5)140(5)
28	1.31	1-10	Decane	43(100)57(82)41(32)71(27)85(17)56(12)
29	1.32	1-10	Hydrocarbon	55(100)41,43(65)56(60)88(55)70(50)83(11)97,111(10)140(5)

TABLE A-68. (Continued)

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
30	1.33	1-10	hydrocarbon	55(100)43(95)56(85)41(62)69(60)70(40)42(30)83, 97(10)140(5)
31	1.51	1-10	Undecane	43(100)57(90)71(43)85(20)
32	1.58	1-10	C ₉ Ketone (T)	71(100)43(65)99(20)55(10)
33	1.60	1-10	naphthalene	128(100)

TABLE A-69. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 29E

OC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Retention Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Match	RI # 103
1	856	ee	Toluene	91(100)92(58)65(18)51(11)	Benzene, Methyl	563
2	875	ee	Octanol	55(100)61(95)63(80)70(58)83(20)112(5)	1-Octanol	640
3	972	ee	Methylcyclohexane	56(100)63(62)61(61)69(70)86(5)91(3)	1-Octene, 2-Methyl	572
4	989	eee	Decane	41(100)55(95)70(70)83(23)97(13)111(6)140(2)	1-Decane	607
5	1002	eee	Propylheptanol	43(100)61(82)57(78)55(71)70(36)85(15)97(6)140(8)142(1)	1-Heptanol, 2-Propyl	520
6	1014	ee	Decane	55(100)61(86)56(78)60(56)97(11)140(12)	1-Decane	607
7	1124	ee	Dimethyldecane	56(100)61(53)69(40)128(11)111(9)168(2)	1-Octene, 2-Methyl	714
8	1163	eee	Dimethyldecane	56(100)55(92)61(89)69(40)83(11)111(9)168(2)	3-Heptene, 2,6-Dimethyl	696
9	1202	eee	Dodecane	55(100)61(95)70(80)83(48)57(28)168(0.5)	1-Dodecane	607
10	1215	ee	Dodecane	55(100)61(70)69(65)83(37)153(20)168(14)170(2)	1-Dodecane	550
11	1239	ee	Methoxy-C ₃ -Benzene	135(100)51(98)121(42)150(33)77(30)	Benzene, 2-Methoxy-1,3,5-Trimethyl	514
12	1297	ee	C ₈ -H ₂ -N-Subst. - Am. L. Iso	136(100)57(64)63(39)71(20)119(20)149(21)		
13	1302	ee	Isomer of 12	139(100)169(30)120(27)91(20)77(16)		
14	1354	eee	1,1'-Biphenyl	156(100)153(62)132(30)76(26)56(22)155(16)	1,1'-Biphenyl	639
15	1376	eee	Diphenyl Ether + ?	170(100)51(95)77(88)161(91)142(81)169(28)171(13)	Benzene, 1,1'-Diphenyl	548
16	1385	eee	7 + 15	Mixed Spectra		
17	1395	eee	Tetradecane	57(100)63(76)71(58)85(30)97(11)111(4)196(0.3)	Tetradecane	697
18	1405	eee	Tetradecane	55(100)61(79)69(56)83(36)97(25)111(9)196(1)	1-Tetradecane	810
19	1416	ee	C $\geq$ 14 Alkane	63(100)57(96)71(70)55(55)85(36)168(1.9)167(1.8)		
20	1467	ee	C $\geq$ 14 Alkane	57(100)63(90)71(78)61(58)85(35)99(8)139(6)168(8)	Pentadecane	735
21	1502	ee	Pentadecane	Same as Above		
22	1540	ee	C $\geq$ 15 Alkane	55(100)60(81)61(69)87(41)97(20)111(21)226(1)	6-Tetradecene, 7-Methyl-	783
23	1560	eee	C $\geq$ 15 Alkane	56(100)69(69)61(62)81(25)111(15)226(0.4)	6-Tetradecene, 7-Methyl-	778
24	1566	ee	C $\geq$ 15 Alkane	56(100)61(36)57(36)69(32)70(32)83(12)97(8)156(1)	1-Pentadecane	691
25	1591	eee	Hexadecane	70(100)55(86)61(65)87(40)97(25)111(11)125(4)	1-Hexadecane	828
26	1604	eee	Hexadecane	57(100)63(75)71(63)55(58)61(55)85(30)	Hexadecane	577
27	1615	ee	Hexadecane	55(100)61(70)69(59)87(46)97(30)111(11)125(5)226(1)	1-Hexadecane	822
28	1606	ee	Hexadecane	55(100)61(96)63(81)57(59)69(69)83(55)97(35)111(16)168(1)	1-Hexadecane	782
29	1702	ee	Heptadecane	57(100)63(90)61(60)71(79)55(55)85(35)182(1.5)	Heptadecane	727
30	1717	ee				

TABLE A-69. (Continued)

QC Peak No.	Retention Index	Amount, μg	Typical Identification	Characteristic ions in Mass Spectrum	Most Reasonable Chemical Name	RT, μmin
31	1757	ee	C $\geq$ 17 Alkene	56 (100) 41 (31) 69 (51) 83 (29) 77 (18) 111 (20) 126 (7) 136 (3) 154 (7)	6-Tridecene, 7-Methyl	757
32	1764	ee	C $\geq$ 17 Alkene	56 (100) 41 (47) 70 (36) 69 (34) 83 (15) 97 (10) 111 (6)	1-Octene, 3,7-Dimethyl-	769
33	1789	ee	C $\geq$ 17 Alkene	70 (100) 55 (66) 41 (54) 83 (28) 97 (19) 111 (9) 125 (4)	1-Undecene, 2-ethyl	575
34	1802	ee	Octadecene	55 (100) 57 (85) 41 (82) 43 (78) 60 (70) 83 (71) 97 (55) 111 (23)	1-Octadecene	775
35	1816	ee	C $\geq$ 18 Alkene	57 (100) 43 (80) 35 (62) 71 (82) 41 (60) 83 (35) 97 (22) 111 (11)		
36	1876	ee	C $\geq$ 18 Alkene	37 (100) 55 (95) 41 (83) 43 (84) 71 (60) 83 (38) 97 (26) 140 (2)		
37	1955	ee	Heptadecanol	55 (100) 41 (66) 43 (84) 69 (72) 82 (63) 97 (42) 111 (20) 125 (8) 196 (0.3)	1-Heptadecanol	820
38	1966	ee	C $\geq$ 19 Alkene	57 (100) 43 (87) 41 (52) 71 (69) 85 (41) 99 (10) 111 (6) 127 (4)		
39	1987	ee	C $\geq$ 19 Alkene			
40	1993	ee	Eicosenes	56 (100) 35 (67) 37 (64) 41 (53) 69 (56) 83 (36) 97 (23) 111 (10) 126 (9)		
41	2003	ee	C $\geq$ 20 Alkene	56 (100) 37 (37) 35 (54) 41 (50) 70 (41) 83 (17) 97 (11) 111 (8)		
42	2155	ee	C $\geq$ 20 Alkene	55 (100) 37 (89) 43 (83) 41 (79) 69 (71) 83 (75) 97 (62) 111 (27) 125 (12)	1-Tridecene	774
43	2196	ee	C $\geq$ 21 Alkene	57 (100) 43 (86) 55 (72) 41 (63) 71 (62) 85 (35) 97 (20) 111 (13)		
44	2292	ee	C $\geq$ 22 Alkene	55 (100) 37 (74) 43 (84) 69 (73) 83 (64) 97 (46) 111 (21)		
45	2357	ee	C $\geq$ 23 Alkene	56 (100) 37 (74) 55 (72) 69 (58) 83 (37) 97 (20) 111 (19)		
46	2398	ee	C $\geq$ 23 Alkene	55 (100) 41 (79) 43 (80) 57 (88)		
47	2553	ee	Docosanol	55 (100) 43 (89) 41 (78) 69 (72) 83 (89) 97 (50) 111 (22) 125 (10)	1-Docosanol	673
48	2750	ee	C $\geq$ 27 Alkene	56 (100) 37 (78) 55 (73) 69 (59) 83 (37) 97 (30) 111 (20) 126 (7) 136 (7)		
49	2849	ee	C $\geq$ 29 Alkene	56 (100) 37 (85) 55 (79) 69 (65) 83 (40) 97 (29) 111 (23) 195 (1.3)		

TABLE A-70. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 29E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Typical Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Match	R.I. $\pm 10^3$
1	910	***	C $\geq$ 6 Fatty acid	76(100)43(83)59(47)87(46)99(23)101(11)	Pentanoic acid, 3-methyl, methyl ester	548
2	1052	**	C $\geq$ 7 Fatty acid	76(100)43(61)41(40)59(23)101(21)127(5)	Hexanoic acid, 5-methyl, methyl ester	567
3	1088	**	Benzoic acid	105(100)77(90)51(76)136(27)	Benzoic acid, methyl ester	575
4	1095	**	Methylphenol	107(100)108(90)77(58)79(50)51(74)63(17)	Phenol, 2-methyl	535
5	1166	**	Benzoic acid	91(100)65(26)150(19)43(11)	Benzoic acid, methyl ester	535
6	1232	**	Methoxy C ₈ -alkylbenzene	135(100)91(69)121(42)150(32)51(24)65(20) 117(41)	Benzoic acid, methyl ester	546
7	1250	**	C $\geq$ 10 Fatty acid	74(100)41(66)43(38)101(33)59(26)155(3)	Benzoic acid, methyl ester	546
8	1386	**	Diphenyl ether	51(100)77(63)141(66)170(65)65(32)115(32)162(44)171(8)	Benzoic acid, methyl ester	513
9	1462	**	C $\geq$ 11 Fatty acid	103(100)43(98)71(57)79(46)55(31)81(26)127(3)	Benzoic acid, methyl ester	572
10	1496	**	C $\geq$ 11 Fatty acid	76(100)87(57)41(48)55(34)115(19)170(20)161(14)183(2)	Benzoic acid, methyl ester	545
11	1685	**	C $\geq$ 16 Fatty acid	55(100)41(95)169(32)74(50)87(31)132(7)196(6)	Tetradecanoic acid, 3-hydroxy, methyl ester	609
12	1911	**	Hexanoic acid	76(100)87(63)43(33)55(38)163(12)	Hexanoic acid, methyl ester	490
13	2080	**	Octadecanoic acid	61(100)55(98)69(50)76(47)87(28)180(2)	11-Octadecanoic acid, methyl ester	500
14	2086	**	Octadecanoic acid	55(100)69(53)76(44)87(26)98(16)266(1)	Benzoic acid, methyl ester	697
15	2111	**	C $\geq$ 18 Fatty acid	76(100)43(64)87(62)55(42)163(10)198(2)185(1)	10-Undecanoic acid, methyl ester	656
					Benzoic acid, methyl ester	590
					Benzoic acid, methyl ester	873

TABLE A-71. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 29E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Typical Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Match	R.I. $\pm 10^3$
1	1123	**	Diethylpyridine	106(100)121(60)77(13)79(8)	Pyridine, 3-ethyl-5-methyl	496
2	1198	*	Octoniline	129(100)102(22)128(20)136(10)75(10)63(6)	Octoniline	737
3	1215	*	N-Ethyl-N-Toluidine or C ₇ -alkylpyridine	120(100)135(36)121(11)91(10)77(9)106(6)		
4	1293	**	Diethylpyridine	136(100)149(38)119(20)91(10)77(7)65(3)		

TABLE A-72. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 30VE

GC Peak No.	Relative Retention Time	Amount, μ g/l	Terpene Identification	Characteristic Ions in Mass Spectrum
1	0.10	----	Air	44(100)
2	0.10	1-10	Buter	41(100)34(70)
3	0.10	1-10	Acetone +	43(100)58(50)101(30)103(10)101(2)
		1-10	Trichlorofluoromethane	
4	0.11	1-10	Dichloroethylene	61(100)36(67)38(50)
5	0.12	1-10	Dichloromethane	49(100)
6	0.21	1-10	Methyl cyclopentane	56(100)41(62)48(60)44(4)
7	0.22	1-10	1,1,1-Trichloroethane	97(100)81(66)99(65)63(22)117,119(12)
8	0.33	1-10	Trichloroethylene	95(100)130(60)132(70)
9	0.70	1-10	Tetrachloroethane	129(100)131(95)144(95)
10	0.89	1-10	C ₆ Alkyl benzene	91(100)106(50)
11	1.00	(8)-	L.S.	75(100)
12	1.18	1-10	C ₆ Alkyl benzene	105(100)120(30)
13	1.19	1-10	C ₆ Alkyl benzene	105(100)120(30)
14	1.21	1-10	C ₆ Alkyl benzene	105(100)120(31)
15	1.31	1-10	C ₆ Alkyl benzene	105(100)120(23)
16	1.32	1-10	Methyl styrene	117(100)118(50)115(36)91(20)
17	1.37	1-10	C ₆ Alkyl benzene (diethyl) C ₁₀ H ₁₄	105(100)119(85)91(30)134(25)
18	1.38	1-10	C ₆ Alkyl benzene	105(100)57(60)118(25)134(15)
19	1.39	1-10	C ₆ Alkyl benzene (ethyl dimethyl)	119(100)91(30)134(20)
20	1.40	1-10	C ₆ Alkyl benzene (methyl propyl)	105(100)134(12)
21	1.44	1-10	C ₆ Alkyl benzene (ethyl dimethyl)	105(100)91(28)134(20)
22	1.47	1-10	C ₆ Alkyl benzene (ethyl dimethyl)	119(100)91(30)105(22)134(15)
23	1.50	1-10	C ₆ Alkyl benzene (n-trimethyl)	119(100)91(25)134(20)
24	1.51	1-10	C ₆ Alkyl benzene	119(100)91(22)134(20)
25	1.55	1-10	Ethyl styrene C ₁₀ H ₁₂	117(100)115(30)

TABLE A-73. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 30E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Reference Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Benzene Match Compound	RI, ± 10
1	863	oo	Toluene	91 (100) 91 (58) 65 (14) 51 (10)	Benzene, Methyl-	943
2	889	ooo	Ethylbenzene	91 (100) 106 (23) 51 (16) 65 (14) 77 (12)	Benzene, Ethyl	942
3	883	ooo	O-xylene	91 (100) 106 (36) 77 (16) 91 (15) 65 (10)	Benzene, 1,2-Dimethyl	940
4	897	ooo	P-xylene	91 (100) 106 (36) 77 (16) 51 (17) 65 (11) 63 (10)	Benzene, 1,4-Dimethyl	933
5	908	oo	2-Butoxyethanol	57 (100) 45 (53) 41 (52) 87 (18)	Ethanol, 2-Butoxy	886
6	934	oo	C ₃ -alkylbenzene	91 (100) 65 (18) 120 (13) 51 (13)	Benzene, Propyl	945
7	942	oo	C ₃ -alkylbenzene	105 (100) 120 (37) 77 (20) 91 (17) 79 (16) 51 (13)	Benzene, 1-Ethyl-2-methyl	901
8	948	oo	C ₃ -alkylbenzene	105 (100) 120 (37) 91 (18) 77 (23) 51 (16) 63 (10) 65 (10)	Benzene, 1,3,5-Trimethyl	975
9	957	oo	C ₃ -alkylbenzene	105 (100) 120 (38) 77 (26) 79 (19) 51 (16) 65 (12) 63 (11)	Benzene, 1-Ethyl-2-methyl	940
10	976	ooo	C ₃ -alkylbenzene	105 (100) 120 (36) 77 (18) 91 (16) 51 (14) 79 (13) 65 (9) 63 (8)	Benzene, 1,2,4-Trimethyl	959
11	1002	oo	C ₃ -alkylbenzene	105 (100) 120 (33) 77 (19) 91 (15) 51 (16) 79 (16) 65 (9) 63 (9)	Benzene, 1,2,4-Trimethyl	956
12	1011	oo	Methylstyrene	117 (100) 118 (57) 91 (32) 63 (26) 51 (22)	Benzene, 1-Ethyl-4-methyl	968
13	1017	oo	C ₃ -alkylbenzene	115 (100) 116 (90) 63 (32) 89 (22) 117 (16)	Benzene, 1,2-Propadienyl	915
14	1029	oo	?	57 (100) 59 (26) 115 (14)	Propane, 1-(1,1-Dimethyl ethoxy)-2-methyl	903
15	1039	oo	C ₆ -alkylbenzene	119 (100) 134 (29) 91 (40) 105 (21) 77 (22) 51 (16) 65 (12) 63 (10)	Benzene, 2-Ethyl-1,4-Dimethyl	923
16	1057	oo	C ₆ -alkylbenzene	119 (100) 91 (33) 134 (23) 77 (20) 51 (15) 65 (11) 63 (10)	Benzene, 2-Ethyl-1,4-Dimethyl	932
17	1064	oo	C ₆ -alkylbenzene	119 (100) 91 (33) 134 (27) 107 (22) 77 (17) 51 (13) 65 (12) 63 (10)	Benzene, 1-Ethyl-2-(1-methyl ethyl)	911
18	1082	oo	C ₆ -alkylbenzene	119 (100) 134 (38) 91 (30) 77 (17) 91 (12) 65 (11) 63 (8)	Benzene, 1,2,4,5-Tetramethyl	922
19	1099	oo	C ₆ -alkylbenzene	119 (100) 134 (36) 91 (31) 77 (17) 91 (14) 65 (11) 63 (8)	Benzene, (1-Ethyl, Propyl)	937
20	1122	oo	Ethylstyrene	117 (100) 91 (44) 132 (29) 51 (26) 63 (18) 65 (17)	Benzene, 1-Ethyl-4-methyl	944
21	1128	oo	Ethylstyrene	117 (100) 115 (60) 138 (31) 91 (23) 63 (18) 65 (16) 77 (16)	Benzene, 1-Ethyl-4-methyl	941
22	1133	oo	C ₆ -alkylbenzene	119 (100) 134 (36) 91 (30) 51 (18) 63 (18) 65 (18)	Benzene, 1,2,4,5-Tetramethyl	944
23	1151	oo	Naphthalene	128 (100) 102 (16) 51 (10) 63 (14) 129 (10)	Naphthalene	918
24	1164	oo	C ₅ -alkylbenzene	133 (100) 148 (24) 77 (20) 119 (17) 105 (18) 51 (15) 91 (15) 65 (10)	Benzene, 1-Ethyl-3-(1-methyl ethyl)	915
25	1261	oo	Methyl naphthalene	162 (100) 141 (89) 115 (60) 63 (20) 51 (12)	Naphthalene, 2-methyl	985
26	1276	oo	Methyl naphthalene	162 (100) 141 (86) 115 (63) 63 (22) 51 (13)	Naphthalene, 2-methyl	913
27	1457	oo	?	57 (100) 71 (25) 167 (31) 165 (27) 137 (13)	3,6-Octadecadienoic Acid, Methyl Ester	925

TABLE A-74. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 30E

GC Peak No.	Retention Time, min	Amount, μ g/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Mass Spectrometric Search Compound	R.I. $\times 10^3$
1	.997	o	Diethyl aniline	106(100)121(40)120(20)77(26)79(18)	Pyridine, 3-Ethyl-4-methyl	639
2	1.063	oo	7	100(100)42(14)56(15)70(14)101(6)145(5)	Urea, Triethyl Nitroso-	348

TABLE A-75. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 31VI

GC Peak No.	Retention Time, min	Amount, μ g/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	oo	Air	44(100)
2	.16	1-10	Acetone	43(100)58(30)
3	.16	1	Diethyl ether	39(100)45(96)74(55)
4	.17	1-10	Dichloromethane	59(100)84(52)86(35)
5	.17	10-20	Chloroprene	41(100)39(68)76(35)55, 78(12)
6	.23	<1	Chloroform	83(100)85(67)
7	.23	<1	Dibutyl ether or Dipropyl ether	45(100)41(43)33(18)59(10)89(4)
8	.25	<1	Tetrahydrofuran 6 7	42(100)41(49)55(57)39(33)71(37)90(12)
9	.26	<1	1,1,1-trichloroethane	97(100)93(67)61(64)118(17)
10	.29	<1	Benzene	78(100)
11	.35	<1	Dichloropropane	63(100)62(75)41(66)39(50)65(10)77(27)76(26)
12	.36	<1	Trichloroethylene	95(100)130(90)132(87)97(62)
13	.40	<1	1,1,2,2-tetrachloroethane	131(100)166(52)129(78)184(67)
14	1.00	-(0)	I.S.	75(100)77(33)

TABLE A-76. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 31VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Terpene Identification	Characteristic Ions in Mass Spectrum
1	0.14	---	Air	44(100)
2	0.15	1-10	Butene	41(100) 56(40)
3	0.17	10-100	Acetone	43(100) 58(25)
4	0.23	10-100	Methyl ethyl ketone	43(100) 72(20)
5	0.29	1-10	1,1,1-Trichloroethane	97(100) 98(70) 61(45) 117, 119, 121
6	0.31	1-10	Methyl isopropyl ketone	43(100) 86(12) 41(11) 71(3)
7	0.31	1-10	Benzene	78(100)
8	0.33	1-10	C_7H_{14} , e.g., 2,3-Dimethyl-1-pentene	41(100) 69(95) 55(45) 70(35) 83(20) 98(10)
9	0.45	1-10	Unknown hydrocarbon	81(100) 41(82) 67(65) 53(60) 79(50) 96(48)
10	0.50	1-10	Methyl isobutyl ketone	43(100) 58(30) 57, 41(20) 85(12) 100(5)
11	0.57	1-10	C_7H_{12} , e.g., Methyl heptadiene	81(100) 79(50) 96(48) 53(47) 41(40)
12	0.59	1-10	C_7H_{12}	81(100) 79(52) 96(45) 53, 41(40)
13	0.62	1-10	C_8H_{16} , e.g., Dimethyl heptene	69(100) 41(88) 55(40) 70(35) 112(30)
14	0.66	1-10	Unknown	57(100) 41(32) 114(11) 85(5) 71(3)
15	0.70	1-10	1,1,1,2-Tetrachloroethane + unknown	43(100) 57(38) 85(30) 41(28) 72(22) 79(31) 131(23) 166(2)
16	0.72	10-100	C7 Ketone, e.g., 2,4-Dimethyl-3-pentene	43(100) 71(30) 41(12) 55(10) 70(9) 86(8)
17	0.76	1-10	3-Methyl-2,4-pentanedione (T)	43(100) 72(28) 71(15) 99(3) 114(3)
18	0.82	1-10	4,4-Dimethylheptane (T)	43(100) 85(30) 41(25) 71(20)
19	0.83	1-10	Ethyl butylaldehyde (T)	43(100) 72(15)
20	0.86	10-100	C8 Ketone, e.g., 4-Methyl-2-heptanone (T)	43(100) 58(93) 91(30) 57(28) 41(22) 85(15)
21	0.88	10-100	C_7 Alkyl benzene	91(100) 106(35)
22	0.96	>100	Cyclooctatetraene (T)	104(100) 78(50) 103(40) 51(33) 77(30) Big One
23	0.97	1-10	Trimethyl cyclohexane (T)	109(100) 67(68) 91(50) 124(20)
24	1.04	>100	Unknown	69(100) 43(85) 41(70) 86(50) 57(30)
25	1.07	10-100	C_7 Alkyl benzene	105(100) 120(25)
26	1.19	1-10	Unknown	67(100) 109(95) 126(40)
27	1.23	1-10	Unknown	43(100) 71(95) 70(20) 41(18)
28	1.29	>100	2-Ethyl-1-hexanol	57(100) 43(51) 41(38) 55(35) 89(23) 83(12) 97(2)

TABLE A-77. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 31E

GC Peak No.	Retention Time, min	Amount, μ g/l	Typical Identification	Characteristic Ion in Mass Spectrum	Most Reasonable Structure Match Compound	E.I. # 103
1	807	ooo	Heptane	43(100)57(60)71(56)78(15)100(10)	Heptane	648
2	818	ooo	Methylcyclohexane	83(100)55(97)96(39)140(39)56(44)	Cyclohexane, Methyl-	583
3	825	oo	C $\geq$ 8 Alkene	43(100)57(76)69(70)85(28)58(8)1.4(1)	Hexane, 3,4-Dimethyl	389
4	850	oo	Toluene	91(100)92(80)85(22)63(15)51(13)30(9)	Benzene, Methyl	542
5	855	oo	C $\geq$ 8 Alkene	43(100)85(66)57(69)73(22)99(6)114(2)		
6	864	oo	Alkyl Ether ?	43(100)59(53)85(23)99(15)100(0.6)		
7	869	oo	Ethylbenzene	91(100)106(25)107(2)	Benzene, Ethyl	749
8	883	ooo	Styrene	104(100)78(68)103(48)57(36)105(8)	Benzene, Ethenyl	622
9	924	ooo	C $\geq$ 9 Alkene	43(100)61(98)69(96)94(68)103(2)104(1)	Hexane, 2,3,3,3-Tetra-methyl	619
10	935	ooo	C $\geq$ alkylbenzene	105(100)120(7)77(27)79(23)51(22)43(17)	Benzene, (1-Methyl Ethyl)-	661
11	982	ooo	C $\geq$ alkylbenzene + ?	57(100)77(96)41(86)105(69)106(65)120(1)125(1)		
12	1031	ooo	Methylheptanol	57(100)43(56)55(80)41(78)63(70)50(83)84(32)97(12)	1-Heptanol, 6-Methyl-	898
13	1081	oo	Alkyl-Alcohol C $\geq$ 8	55(100)61(99)56(90)69(60)84(61)122(1)	1-Octanol	772
14	1082	oo	Alkyl-Alcohol or Alkene	43(100)55(77)41(72)57(63)69(56)83(26)121(21)	1-Heptanol, 6-Methyl	637
15	1087	oo	Alkyl-Alcohol or Alkene	57(100)61(73)69(70)55(50)83(12)111(6)	1-Heptanol, 6-Methyl-	616
16	1108	oo	Alkyl-Alcohol or Alkene	69(100)55(98)41(87)83(29)97(16)	4-Decene	670
17	1119	oo	Alkyl-Alcohol or Alkene Mixture	43(100)59(55)101(52)57(50)85(26)83(19)127(6)		
18	1137	oo	Alkyl-Alcohol or Alkene	43(100)65(69)73(66)55(65)87(38)131(0.6)	3-Heptanol, 2,4-Dimethyl	577
19	1164	oo	Alkyl-Alcohol or Alkene	55(100)61(70)69(54)57(62)97(30)83(26)115(3)	1-Heptanol, 6-Methyl-	746
20	1187	oo	C $\geq$ 12 Alkene	41(100)55(94)69(95)83(68)57(65)	1-Pentadecene, 2-Methyl-	736
21	1193	oo	Alkyl-Alcohol or Alkene	57(100)61(81)69(83)56(59)55(57)112(12)	1-Decanol	787
22	1201	oo	Alkyl-Alcohol or Alkene	55(100)61(80)69(76)83(23)112(17)111(15)	Isocetene, (Ethenylmethyl)-	540
23	1207	oo	Alkyl-Alcohol or Alkene	69(100)63(79)41(77)70(55)55(53)112(16)	1-Heptene, 6-Methyl	623
24	1217	oo	Alkyl-Alcohol or Alkene	55(100)61(66)83(39)69(21)97(18)	1-Nonene	527
25	1229	oo	1-Phenyl-1-Propanol	77(100)105(99)51(51)136(2)		
26	1361	oo	Subst.-Styrene	104(100)78(28)51(13)178(2)165(1)		
27	1690	o	?	91(100)57(73)43(68)61(32)71(66)130(17)208(6)		
28	1718	oo	Subst.-Styrene	104(100)78(22)51(10)178(6)179(3)		
29	2408	oo	Subst.-Benzene	91(100)117(20)65(14)77(12)51(6)207(5)208(2)		
30	2496	oo	Subst.-Benzene	91(100)129(66)207(26)105(23)177(20)208(12)208(6)		

TABLE A-77. (Continued)

GC Peak No.	Retention Time, min	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Responsible Biomarker Molecules	
					Compound	RI ± 10°
31	2516	ccc	Subst. - Benzene	91 (100) 129 (63) 207 (23) 77 (19) 206 (10) 208 (4)		
32	2539	cc	Subst. - Benzene	91 (100) 129 (10) 207 (30) 105 (25) 77 (22)		
33	2611	cc	Subst. - Benzene	91 (100) 129 (40) 104 (37) 77 (20) 85 (16) 207 (9) 208 (9)		

TABLE A-78. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 31E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Volatiles Identification	Characteristic Ions in Mass Spectrum	Main Reasonable Chemical Match	Elution
1	816	oo	C ₂₋₆ Fatty acid	74(100)42(31)59(28)99(15)101(14)	Pentanoic acid, 3-methyl-methyl ester	541
2	842	o	C ₂₋₆ Fatty acid	74(100)87(63)55(31)54(31)48(27)42(22)99(30)104(22)	Pentanoic acid, 4-methyl-methyl ester	477
3	852	oo	C ₂₋₆ Fatty acid	88(100)63(36)87(30)101(30)69(25)74(19)111(6)	Heptanoic acid, 2,6-dimethyl, methyl ester	475
4	868	oo	C ₂₋₇ Fatty acid	88(100)57(33)41(27)87(19)69(17)113(6)115(5)		
5	878	oo	C ₂₋₇ Fatty acid	88(100)57(26)41(18)59(16)87(11)115(6)113(5)		
6	882	oo	C ₂₋₇ Fatty acid	74(100)87(74)43(41)59(35)69(23)101(32)112(20)129(2)	Heptanoic acid, methyl ester	419
7	893	oo	C ₂₋₇ Fatty acid	74(100)63(36)59(27)73(26)101(26)113(14)	Hexanoic acid, 5-methyl, methyl ester	434
8	900	oo	C ₂₋₇ Fatty acid	87(100)74(99)55(67)41(46)73(41)59(36)115(28)113(24)		
9	902	oo	C ₂₋₇ Fatty acid	87(100)102(61)55(30)57(22)115(19)130(10)143(2)		
10	912	oo	C ₂₋₇ Fatty acid	87(100)107(64)116(44)57(35)127(6)129(4)		
11	928	ooo	C ₂₋₇ Fatty acid	88(100)101(32)57(28)69(24)41(23)129(8)127(5)		
12	940	oo	C ₂₋₇ Fatty acid + 7	74(100)101(34)63(26)59(20)88(19)127(6)143(2)		
13	942	oo	C ₂₋₇ Fatty acid + 7	69(100)41(54)87(56)55(43)84(36)116(18)		
14	948	oo	C ₂₋₇ Fatty acid	88(100)57(62)41(37)76(42)111(26)127(15)143(12)		
15	957	ooo	C ₂₋₈ Fatty acid	87(100)102(70)41(38)55(36)57(34)69(28)130(12)		
16	974	ooo	C ₂₋₈ Fatty acid	74(100)87(37)55(34)63(28)609(23)115(13)127(11)		
17	981	ooo	C ₂₋₈ Fatty acid	74(100)87(65)41(30)69(34)101(32)55(27)59(25)127(14)129(8)		
18	994	ooo	C ₂₋₈ Fatty acid	74(100)101(32)59(16)69(14)87(11)127(10)143(1)		
19	1005	oooo	Benzoic acid	74(100)55(74)115(75)83(68)87(64)59(34)109(26)127(12)	Benzoic acid, M.E.	572
20	1081	oo	C ₂₋₈ Fatty acid	105(100)77(66)136(56)51(21)115(4)	Hexanoic acid, methyl ester	438
21	1069	oo	C ₂₋₈ Fatty acid	74(100)101(40)41(30)55(28)115(14)123(10)141(6)		
22	1089	oo	C ₂₋₉ Fatty acid	87(100)74(58)55(48)57(44)99(18)115(14)141(9)157(2)		
23	1097	oo	C ₂₋₉ Fatty acid + 7	88(100)101(99)87(82)41(40)69(48)43(41)129(20)141(7)143(6)	Undecanoic acid, 2-methyl, methyl ester	506
24	1105	oo	C ₂₋₉ Fatty acid	87(100)101(88)74(76)55(65)102(73)111(46)143(44)		
25	1119	oo	C ₂₋₉ Fatty acid	88(100)101(48)69(37)43(37)55(36)129(19)143(10)	Heptanoic acid, 2-ethyl	456
26	1135	oo	C ₂₋₉ Fatty acid + 7	74(100)55(62)47(61)41(33)97(40)115(20)129(34)143(4)		
27	1159	oo	C ₂₋₉ Fatty acid	74(100)88(79)55(27)87(20)129(17)143(17)155(7)157(3)	Decanoic acid, methyl ester	450
28	1163	oo	C ₂₋₉ Fatty acid	74(100)55(46)83(40)88(37)115(20)87(25)157(18)		
29	1166	oo	C ₂₋₉ Fatty acid	74(100)101(64)55(26)69(24)137(8)155(4)157(3)		
				74(100)115(18)55(26)143(22)157(20)143(8)		

TABLE A-78. (Continued)

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Name	E.I. $\times 10^3$
30	1169	**	C $\geq$ 9 Fatty acid	74(100)101(49)68(26)55(19)59(18)163(8)	Hexanoic acid, 5-methyl-methyl ester	610
31	1174	**	C $\geq$ 9 Fatty acid	74(100)87(95)55(55)69(47)113(30)143(18)155(8)157(4)	Tetradecanoic acid, 12-methyl-methyl ester	415
32	1176	**	C $\geq$ 9 Fatty acid	74(100)101(83)55(30)89(29)87(30)143(7)155(6)171(2)		
33	1186	**	C $\geq$ 9 Fatty acid + ?	74(100)101(86)55(33)97(22)87(20)143(5)155(4)157(3)		
34	1190	***	C $\geq$ 9 Fatty acid	87(100)74(67)55(32)97(24)143(8)155(4)157(2)		
35	1199	***	C $\geq$ 9 Fatty acid	87(100)74(54)55(44)57(38)97(22)155(4)		
36	1203	**	C $\geq$ 10 Fatty acid	87(100)74(54)55(44)113(15)143(5)155(6)171(1)		
37	1211	**	C $\geq$ 10 Fatty acid	101(100)87(99)75(81)102(67)89(62)113(37)155(16)142(6)		
38	1215	**	C $\geq$ 10 Fatty acid	74(100)87(60)97(60)68(57)55(54)41(47)129(42)137(17)		
39	1217	**	C $\geq$ 10 Fatty acid	74(100)55(80)83(65)87(39)111(35)143(28)		
40	1221	**	C $\geq$ 10 Fatty acid	74(100)115(54)55(48)87(40)83(34)137(14)143(3)		
41	1222	**	C $\geq$ 10 Fatty acid	129(100)97(66)69(65)87(56)74(47)41(41)55(40)137(11)	Octadecanoic acid, dimethyl ester	420
42	1226	**	C $\geq$ 10 Fatty acid	129(100)97(66)69(60)74(56)87(55)55(43)137(11)		
43	1238	**	C $\geq$ 10 Fatty acid	111(100)83(99)74(82)55(81)87(67)143(56)154(4)	Dodecanoic acid, 10-methyl-methyl ester	596
44	1911	**	Hexanoic acid	74(100)87(85)55(28)143(24)227(6)		
45	1978	**	?	134(100)107(32)79(29)57(54)166(21)167(21)234(5)		
46	2080	**	C $\geq$ 18 Fatty acid	55(100)68(72)74(70)83(62)87(54)97(56)180(10)264(8)	10-Octadecanoic acid, methyl ester	443
47	2111	**	C $\geq$ 18 Fatty acid	74(100)87(86)142(31)55(29)199(14)	Heptadecanoic acid, methyl ester	537
48	2230	**	Subst. phanthrene carboxylic acid	121(100)91(24)105(19)241(3)318(2)		
49	2512	**	Subst. phanthrene carboxylic acid	121(100)81(35)107(30)189(27)302(3)303(2)347(1)		

TABLE A-79. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 31E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Name	E.I. $\times 10^3$
			Neutral compounds were also concentrated into basic fraction.			
			No basic compounds were identified in this fraction.			

TABLE A-80. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 32VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.19	---	Air	44(100)
2	0.24	10-100	Dichloromethane	49(100)
3	0.25	10-100	Cyclopentadiene	66(100) 65(70) 40(40)
4	0.25	1-10	Cyclopentene	67(100) 68(45) 53(20)
5	0.26	1-10	1-Pentene	42(100) 55(35) 70(25)
6	0.30	10-100	Chloroform	83(100) 85(70) 82(40) 47(38) 53(30) 85(10)
7	0.33	1-10	Benzene	78(100)
8	0.35	1-10	C_6H_8 eg Cyclohexadiene	79(100) 80(50) 77(45)
9	0.35	1-10	C_6H_8 eg Cyclohexadiene	79(100) 80(55)
10	0.36	1-10	C_6H_{10} eg 2,4-Hexadiene	67(100) 82(22) 41(21)
11	0.40	1-10	Cyclohexane	67(100) 54(70) 82(35) 41(33)
12	0.43	1-10	Bromodichloromethane	83(100) 85(70) 47(28) 127, 129, 131
13	0.44	1-10	Tetramethyl butane (T)	57(100) 41(32) 56(30) 43(22)
14	0.59	1-10	Unknown	43(100) 71(48) 70(30) 84(29) 91(18) 94(13) (Weak spectrum)
15	0.83	1-10	C_8H_{12} eg 4-Vinylcyclohexene	54(100) 79(60) 66(40) 80(30)
16	1.34	1-10	Dicyclopentadiene	66(100) 65(20)

TABLE A-81. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 32E

GC Peak No.	Retention Index	Amount, µg	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Benzene Match Compound	R.I. ± 10 ³
1	862	oo	C ₉ -alkylbenzene	105(100)91(46)51(38)120(36)77(35)		
2	867	oo	C ₉ -alkylbenzene	105(100)91(26)51(32)120(36)77(38)	Benzene, 1-ethyl-2-methyl	431
3	881	oo	?	66(100)51(11)78(27)62		
4	948	oo	Indene	115(100)116(90)89(22)83(33)51(20)	1H-Indene	398
5	957	oo	Methylindene	115(100)130(73)51(35)83(29)77(26)117(29)131(13)	1H-Indene, 3-methyl	368
6	972	oo	Methylindene (C ₁₀ H ₁₀) + C ₄ -alkylbenzene	115(100)130(82)129(82)51(28)83(26)77(20)		
7	1151	oo	Naphthalene + ?	128(100)102(15)51(16)83(16)76(12)129(12)	Acetone	559
8	1191	ooo	Tetrahydrothiophene 1,1-dioxide C ₄ H ₆ O ₂ S + Sulfur-containing compound	41(100)56(56)55(50)120(16)84(8)	Thiophene, tetrahydro-1,1-dioxide	614
9	1283	oo	Methylnaphthalene	142(100)141(89)115(61)83(20)89(12)51(12)143(13)	Naphthalene, 2-methyl	349
10	1276	oo	Methylnaphthalene	142(100)141(94)115(66)83(21)89(12)76(11)143(12)	Naphthalene, 2-methyl	437
11	1288	oo	Dihydro-dimethylnaphthalene	131(100)146(18)115(62)102(32)83(23)51(23)77(22)39(20)	1H-Indene, 2,3-dihydro-Δ ² ,6-dimethyl	362
12	1304	oo	Tetrahydrodimethylnaphthalene	115(100)117(97)160(52)83(41)145(37)91(35)163(31)	Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl	340
13	1398	oo	Alkyl alcohol C ≥ 12	89(100)86(87)43(62)55(46)131(8)174(5)		
14	1433	oo	Subst. alkylbenzene + ?	104(100)77(36)91(25)83(19)51(18)89(15)148(12)		
15	1481	oo	Subst. alkylbenzene ?	117(100)118(92)91(32)77(26)51(11)83(18)162(6)		
16	1553	oo	Mixture ?	98(100)79(71)77(47)70(31)41(29)152(26)175(31)		
17	1633	oo	Subst. alkylbenzene + ?	91(100)77(92)51(60)105(55)130(45)144(40)172(25)190(12)		
18	1700	oo	Subst. alkylbenzene	91(100)77(78)79(71)117(60)143(33)85(40)186(22)204(22)		

TABLE A-82. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 32E

GC Peak No.	Retention Index	Amount, μg	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Benzene Match Compound	RT, $\times 10^3$
1	1078	oo	?	66(100)91(22)65(19)35(16)77(16)121(5)152(6)		
2	1085	oo	?	66(100)91(22)65(20)35(18)77(12)121(5)152(5)		
3	1166	ooo	?	41(100)56(62)35(56)120(38)148(76)64(23)		
4	1280	o	Hydroxybenzoic acid	134(100)106(48)105(47)77(66)166(66)135(38)	Benzoic acid, 2-pyrenyl-4-methyl, methyl ester 564	
5	1321	oo	?	172(100)157(72)97(63)113(50)25(48)79(61)58(36)65(27)		
6	1338	oo	?	95(100)126(90)91(38)77(26)148(16)167(8)		
7	1363	oo	Subst. naphthalene	186(100)59(66)171(60)127(53)139(62)65(21)		
8	1351	oo	Subst. naphthalene	186(100)171(66)111(50)127(66)139(66)59(62)		
9	1356	oo	Subst. naphthalene	186(100)111(66)171(66)59(35)93(31)127(30)155(18)		
10	1381	oo	?	117(100)186(59)111(66)115(62)59(66)77(22)171(25)		
11	1555	oo	?	129(100)128(88)108(39)127(36)151(20)212(6)		
12	1692	oo	?	126(100)79(76)77(56)175(59)167(56)202(7)		

TABLE A-83. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 32E

GC Peak No.	Retention Index	Amount, μg	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Benzene Match Compound	RT, $\times 10^3$
1	1109	o	C ₈ -alkylpyridine	135(100)134(61)120(28)79(16)77(15)91(15)	Pyridine, 6(1,1-dimethyl 8-ethyl)-	283
2	1172	ooo	Mixture, Solfolene + ?	61(100)56(59)35(56)120(50)84(10)148(10)169(3)	Phthalene, Tetracyclo	296
3	1225	o	Dimethylquinoxaline	157(100)115(20)167(13)156(23)158(13)89(8)	Quinoxaline, 2,4-dimethyl	608
4	1232	o	Mixture ?	131(100)121(78)107(52)91(62)77(28)168(66)206(2)	18-Indene-1,1,2-diol, 2,3-dihydro-1-methyl	583

TABLE A-84. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 33VE

GC Peak No.	Relative Retention Time	Amount, μ g/l	tentative identification	Characteristic ions in Mass Spectrum
1	0.13	---	Air	44(100)
2	0.16	<1	Residue	41(100) 56(66)
3	0.16	1-10	Acetone	43(100) 58(25)
4	0.16	1-10	Diethyl ether	58(100) 74(72) 45(70)
5	0.16	1-10	Dichloroethylene	81(100) 96(40) 83(30) 38(28)
6	0.17	10-100	Dichloromethane	49(100)
7	0.17	1-10	Dicyclopentadiene	66(100) 65(70) 40(48)
8	0.21	<1	Methyl ethyl ketone	43(100) 72(20)
9	0.23	1-10	Diisopropyl ether	45(100) 43(64) 87(20) 59(10)
10	0.26	<1	1,1,1-Trichloroethane	87(100) 99(60) 81(40) 117, 119, 121
11	0.26	<1	Benzene	78(100)
12	0.33	1-10	1,2-Dichloropropane	83(100) 82(68) 41(65) 76(40)
13	0.38	<1	Methyl-t-butyl ketone	57(100) 41(70) 43(46) 100(15) 55(10)
14	0.62	<1	C ₁₀ H ₁₆ 98 2,4,4-trimethyl-1,3-pentene	57(100) 41(55) 55(35) 68(10) 87(10) 112(10)
15	0.48	<1	C ₈ H ₁₆	55(100) 87(50) 41(65) 68(25) 112(20)
16	0.63	<1	C ₈ H ₁₆	55(100) 83(80) 41(65) 68(30)
17	0.92	<1	C ₈ Alkyl benzene	91(100) 106(40)
18	1.00	B ~	I 5	75(100)
19	1.21	<1	C ₉ Alkyl benzene	105(100) 120(15)
20	1.23	1-10	C ₉ Alkyl benzene	119(100) 91(28) 134(20)
21	1.44	<1	C ₉ Alkyl benzene	119(100) 91(30) 134(20)

TABLE A-85. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 33E

GC Peak No.	Retention Index	Amount, μg	Typical Identification	Characteristic Ion in Mass Spectrum	Most Reasonable Chemical Name	K.I. $\times 10^3$
1	861	ss	Toluene	91(100) 92(84) 93(24) 51(14) 91(8)	Benzene, Methyl-	540
2	867	ss	Allyl-ether	59(100) 57(40) 41(22) 43(19) 113(13) 97(11)	Propane, 1-(1,1-dimethyl ethoxy)-2-methyl	508
3	870	ss	Ethyl benzene	91(100) 106(48) 105(19) 77(13) 163(10)		
4	895	ss	Allyl-ether	63(100) 61(75) 57(86) 59(76) 35(36) 72(59) 71(62) 101(12)	Notane, tert-butyl isopropyl	519
5	906	ss	C = 9 Alkene $\text{C}_{10}\text{H}_{18}$	67(100) 109(50) 61(44) 63(42) 81(39) 124(18)		
6	998	ss	Allyl alcohol or Alcohol	63(100) 72(64) 57(53) 61(32) 81(39) 85(45) 99(6)	Pinene, 1-(1-butanyloxy)-	631
7	1028	ss	(Methylcyclohexane) $\text{C}_{10}\text{H}_{18}$	61(100) 55(84) 69(54) 85(59) 104(29) 120(6) 140(19)		
8	1034	ss	$\text{C}_{10}\text{-cyclohexanol}$ $\text{C}_{10}\text{H}_{18}\text{O}$	66(100) 109(64) 81(56) 61(50) 62(49) 57(40) 81(58) 124(27) 138(6)	Cyclohexane, 4-sec-butyl	554
9	1048	ss	$\text{C}_{10}\text{-cyclohexanone}$ $\text{C}_{10}\text{H}_{16}\text{O}$	67(100) 95(88) 98(54) 61(67) 81(45) 110(29) 138(33) 139(3)	2-cyclohexen-1-one, 3,4,4-trimethyl-	653
10	1076	ss	$\text{C}_{10}\text{-cyclohexanone}$	127(100) 95(83) 67(50) 61(54) 55(22) 110(19) 138(33) 139(4)	Cyclohexanone, 2-(1-methylindene)-	605
11	1090	ss	$\text{C}_{10}\text{-cyclohexadiene}$	79(100) 77(62) 136(4)	2,3-Cyclohexadien-1-one, 2,4,4-trimethyl	581
12	1223	ss	Allylcyclohexanone	63(100) 61(67) 56(75) 69(52) 86(21) 99(15) 114(13) 124(8)	Cyclohexanone, 4-ethyl	536
13	1277	ss	Mixture ?	56(100) 61(78) 65(76) 55(25) 121(7) 149(2) 140(0.2)		
14	1288	ss	Tenure of 13 ?	56(100) 61(74) 65(85) 118(12) 121(45) 149(5)		
15	1395	ss	?	77(100) 65(99) 91(83) 111(58) 154(35)		
16	1432	ss	Allyl-toluene	61(100) 81(84) 69(85) 86(80) 35(78) 57(75) 165(45) 180(20) 221(3)		
17	1460	ss	?	69(100) 63(62) 61(50) 64(44) 55(37) 127(8) 181(3) 205(2)		
18	1479	ss	?	69(100) 61(58) 55(58) 66(16) 95(18) 177(8)		
19	1548	ss	Nonmethiol	55(100) 56(84) 69(88) 61(60) 86(34) 98(16) 160(7)	1-methanethiol	585
20	1560	ss	Allyl-alcohol	61(100) 70(83) 55(63) 69(57) 83(13) 183(11)	4-methanethiol, 2-ethyl-2-methyl-	649

TABLE A-86. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 33E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum	Most Reasonable Benzene Match Compound	U.I. # 103
1	941	oo	?	37 (100) 101 (40) 51 (24) 116 (28) 71 (20) 137 (7) 87 (6)		
2	997	oo	C ₂ -6 Fatty acid	41 (100) 57 (64) 101 (72) 116 (70) 71 (21) 87 (11) 87 (6) 137 (2)		
3	1004	oo	?	41 (100) 115 (100) 37 (40) 130 (30) 43 (34) 59 (31) 83 (22) 102 (22)		
4	1017	oo	?	64 (100) 55 (26) 91 (10) 87 (16) 121 (6) 132 (3)		
5	1026	oo	Isomer of #4	64 (100) 55 (15) 91 (10) 87 (9) 77 (8) 121 (6) 132 (3)		
6	1037	oo	?	102 (100) 43 (69) 41 (61) 73 (50) 85 (35) 87 (30) 143 (27) 137 (1)		
7	1044	oo	?	80 (100) 79 (40) 35 (14) 91 (10) 65 (5) 135 (3)		
8	1100	oo	Isomer of #4	102 (100) 43 (45) 41 (34) 87 (23) 71 (14) 55 (14) 127 (3) 143 (1)		
9	1119	oo	Isomer of #3	71 (100) 115 (59) 43 (59) 37 (53) 130 (30) 143 (6) 136 (3)		
10	1126	ooo	C ₂ -8 Fatty acid + ?	101 (100) 41 (54) 35 (40) 149 (32) 116 (34) 130 (10) 144 (6) 137 (2)		
11	1132	oo	C ₂ -8 Fatty acid	101 (100) 41 (54) 35 (40) 149 (32) 116 (34) 130 (10) 144 (6)	Benzoic acid, 2-methyl-2-propyl-methyl ester	414
12	1138	oo	?	116 (100) 41 (99) 71 (51) 35 (42) 101 (65) 127 (18) 137 (3) 158 (2)		
13	1187	oo	C ₂ -8 Fatty acid	101 (100) 116 (50) 43 (56) 41 (48) 113 (32) 158 (8) 137 (4)		
14	1342	oo	?	102 (100) 57 (66) 41 (42) 43 (30) 71 (34) 83 (26) 115 (18) 171 (3)		

TABLE A-87. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 33E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum	Most Reasonable Benzene Match Compound	U.I. # 103
1	859	oo	Nethylpyridine	91 (100) 54 (7) 64 (30) 145 (29) 63 (21)	Pyridine, 4-methyl-	607
2	964	oo	Triethylpyridine	121 (100) 120 (31) 79 (22) 77 (14) 106 (19) 122 (10)	Pyridine, 2,3,5-trimethyl	534
3	980	ooo	Triethylpyridine	121 (100) 120 (26) 77 (18) 51 (12) 106 (18) 122 (9)	Pyridine, 2,3,5-trimethyl	438
4	1100	oo	2,6-dimethyl-4-ethylpyridine	135 (100) 134 (66) 120 (30) 91 (16) 79 (16) 77 (14) 136 (10)	Hexanamine, N-(Phenylmethyl)-N-oxide	265
5	1112	oo	C ₅ -allylpyridine (Isomer of #4)	135 (100) 134 (62) 120 (25) 79 (17) 77 (14) 91 (14) 136 (10)	Pyridine, 4-(1,1-dimethyl ethyl)-	233
6	1190	oo	? MW 129	43 (100) 57 (64) 81 (54) 114 (50) 129 (64) 128 (8)		
7	1205	oo	C ₅ -allylpyridine MW 149	148 (100) 149 (46) 150 (43) 121 (18) 91 (9) 77 (10)	7 (18) -Teridione	350
8	1259	oo	Mixture of MW 149	41 (100) 36 (95) 85 (43) 121 (22) 149 (16)		
9	1299	oo	Alkylthiophene	125 (100) 140 (81) 97 (80) 31 (43) 77 (39) 109 (17) 141 (8)	Thiophene, 2-(1,1-dimethyl ethyl)	208

TABLE A-88. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 34VE

GC Peak No.	Retention Time	Amount, µg/l	Testative Identification	Characteristic Ions in Mass Spectrum
1	0.13		Air	44(100)
2	0.14	10-100	C ₄ H ₆	56(100)41(70)55(45)
3	0.16	1-10	Puran	68(100)49(3)
4	0.17	1-10	Dichloromethane	49(100)
5	0.22	10-100	Chloroprene	53(100)88(90)50, 51(48)90(30)
6	0.24	10-100	Dihydrofuran	70(100)41(70)40, 42(40)69(32)
7	0.24	10-100	Chloroprene	53(100)88(75)50(30)51(30)90(90)
8	0.25	1-10	Chlorobutene	55(100)90(50)53(38)92(20)
9	0.27	1-10	Croton aldehyde or dihydro pyron	70(100)41(70)69(45)
10	0.27	1-10	C ₄ H ₆ O + 1,1,1-trichloroethane	70(100)41(68)97(80)99, 101, 117, 119, 122
11	0.29	1-10	Benzene	78(100)
12	0.44	1-10	C ₈ H ₁₆ , n-B., 2,4,4-Trimethyl-1-pentene	57(100)41(48)112(28)97(20)
13	0.48	1-10	C ₈ H ₁₆	97(100)112(40)55(38)69, 41(15)
14	0.51	10-100	Chlorobutene + Dichlorobutene (M126)	63(100)62(98)55(40)96(40)
15	0.55	10-100	Dichlorobutene + Chlorobutene	63(100)62(98)55(48)90(40)
16	0.58	10-100	Dichlorobutene (M124)	75(100)58(50)89(45)77(20)
17	0.61	10-100	1,2-Dichlorobutene (M126)	55(100)77(62)41(48)71(40)96(22)
18	0.61	1-10	Dichlorobutene	55(100)41, 77(80)82, 76(35)90(20)
19	0.90	1-10	C ₈ H ₆ Cl ₂ , n-B., 1,3-Dichloro-2-methylene	88(100)70(50)53(48)90(33) 86, 124, 126, 128
20	0.97	10-100	Propane	
21	1.00	B-	1,4-Dichlorobut-2-ene	75(100)53(70)89(40)88(55)77(33)62(28)124(20), 126, 128
22	1.21	1-10	Tri-isobutene	75(100)
23	1.23	10-100	Unknown	57(100)41(25)97(20)112(15)146(14)
24	1.40	1-10	C ₈ H ₆ Cl ₂ , n-B., (1-Chloromethyl) benzene	97(100)57(55)112(25)41(22)69(20)83(18)168(12)
25	1.58	100	Unknown	105(100)140(50)103(40)77(30)112(25)142(20)
26	1.59	1-10	1,2-Dichloro-cycloocta-1,5-diene (T)	111(100)103(40)88(55)77(40)141(20)176(5)
				88(100)53(40)105(30)141(25)

TABLE A-89. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 34E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Structure Match	E.I. $\Delta 10^\circ$
1	886	oo	Ethylbenzene	59 (100) 43 (96) 91 (80) 106 (24)		
2	896	oo	O-Xylene	91 (100) 106 (71) 59 (32) 37 (30) 43 (28) 77 (26) 92 (16)	Benzene, 1,4-dimethyl	326
3	907	oo	P-Xylene	91 (100) 106 (49) 43 (20) 105 (21) 77 (16) 57 (15)	Benzene, 1,3-dimethyl	486
4	997	oo	1-Propene, 2-methyl trimer	57 (100) 41 (56) 97 (13) 112 (7) 168 (6)		546
5	1007	oo	1-Propene, 2-methyl trimer	97 (100) 57 (98) 41 (77) 69 (40) 83 (26) 112 (23) 168 (10)	1-Propene, 2-methyl, trimer	582
6	1187	ooo	Chloro-7 mixture	123 (100) 35 (90) 70 (86) 77 (54) 95 (30) 105 (23) 158 (7) 160 (2)		
7	1208	oo	Isomer of #6	123 (98) 77 (96) 53 (95) 70 (82) 95 (76) 105 (62) 158 (18) 160 (6)		
8	1212	oo	1-Chloro-5-(1-chloroethyl) cyclohexane	88 (100) 105 (92) 51 (70) 161 (59) 113 (44) 163 (18) 176 (16) 178 (11)	Cyclohexane, 1-chloro-5-(1-chloroethyl)	603
9	1225	oo	Isomer of #8	67 (100) 123 (99) 102 (75) 53 (48) 88 (60) 176 (4) 178 (1)		
10	1231	oo	Isomer of #8	67 (100) 88 (83) 123 (76) 53 (44) 95 (69) 102 (31) 158 (12) 160 (4)		
11	1266	oo	?	63 (100) 112 (92) 97 (63) 89 (40) 67 (39) 125 (15) 146 (12)	1-Heptene, 3-ethyl-3,4-dimethyl	481
12	1284	oo	Allylbenzene C ₂ 10	63 (100) 127 (20) 111 (16) 95 (14) 71 (14) 153 (2) 168 (1)		
13	1311	ooo	1,3-Butadiene, 2-chloro, dimer	88 (100) 55 (96) 105 (60) 161 (58) 91 (45) 163 (18) 176 (11) 178 (10.4)		422
14	1317	oo	1-Propene, 2-methyl-tetramer	57 (100) 41 (36) 55 (16) 97 (10) 83 (8) 113 (8) 160 (1)	1-Propene, 2-methyl, tetramer	546
15	1339	oo	Isomer of #13	57 (100) 41 (34) 55 (32) 97 (31) 70 (28) 112 (18) 176 (1) 178 (0.4)		
16	1351	oo	?	106 (100) 106 (30) 41 (18) 33 (17) 137 (5) 158 (1)		
17	1363	oo	?	106 (100) 77 (75) 157 (61) 91 (58) 51 (48) 159 (20) 180 (3) 186 (2)		
18	1375	oo	?	106 (100) 106 (32) 69 (26) 55 (20) 157 (13) 159 (4)		
19	1393	oo	Acetic acid C ₂ 8 ester	86 (100) 69 (97) 41 (59) 43 (46) 70 (37) 55 (32) 157 (0.4)	Acetic acid, ethyl ester	510
20	1637	oo	Acetic acid C ₂ 9 ester	86 (100) 69 (96) 41 (95) 43 (78) 55 (40) 148 (4) 180 (2) 177 (1)		

TABLE A-90. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 34E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Benzene Deriv. Compound	E.I. # 10 ⁵
1	862	oo	C ≥ 6 Fatty acid	87(100)41(76)59(65)95(36)96(32)126(32)111(9)	4-Pentenoic acid, 2-methyl-, methyl ester	202
2	1017	oo	?	66(100)55(13)91(11)92(5)121(6)152(3)		
3	1026	oo	Methyl cyclohexane-1-carboxylic acid	79(100)67(45)41(44)95(27)122(21)156(26)		
4	1042	oo	?	80(100)79(45)55(15)91(10)135(3)93(3)	3-Oxobutanoic acid, 4-methyl	324
5	1090	oo	?	109(100)68(89)67(76)93(49)136(14)168(4)		
6	1115	oo	?	70(100)55(50)123(49)77(13)95(9)79(7)158(4)		
7	1211	oo	Alkylphenol	94(100)79(79)65(14)121(12)155(10)121(12)152(4)160(3)		
8	1226	oo	Subst. Benzenesulfonic acid	91(100)151(100)65(31)59(23)155(11)185(2)		
9	1263	oo	Subst. Benzenesulfonic acid	91(100)158(27)65(27)59(16)127(16)171(2)		
10	1276	oo	Subst. Benzenesulfonic acid	91(100)151(57)65(27)59(26)77(14)		
11	1316	oo	Benzenesulfonic acid-4-methoxy hydrazide	91(100)127(19)125(18)65(18)151(9)186(3)		
12	1324	ooo	?	95(100)128(78)91(44)77(20)148(10)186(1)188(0.3)		
13	1353	oo	?	151(100)91(56)65(18)155(10)186(5)188(2)		
14	1362	oo	?	91(100)65(18)118(23)151(14)186(18)188(4)		
15	1374	oo	?	91(100)65(26)77(20)154(40)125(29)127(18)186(26)188(10)		
16	1380	oo	?	151(100)91(47)65(20)51(14)155(14)186(8)188(3)		
17	1502	oo	?	145(100)129(9)117(83)115(81)91(86)77(43)		
18	1696	ooo	?	126(100)79(98)175(47)		
19	1716	oo	?	79(100)97(53)77(35)91(30)126(20)87(13)175(41)		
20	1815	oo	C ≥ 15 Fatty acid	74(100)87(76)	Pentadecanoic acid, 14-methyl-, methyl ester	534
21	2383	oo	?	137(100)79(63)77(46)91(44)216(18)191(13)217(8)		
22	2425	oo	?	79(100)137(86)77(63)91(40)43(28)216(18)276(6)		

TABLE A-91. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 34E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Name	RI, ± 10
1	911	ee	?	55(100)121(67)79(66)36(58)42(41)107(16)122(6)		
2	1162	ooo	Mixture ?	123(100)79(84)55(52)77(26)105(20)158(6)		
3	1341	*	1,3,5-Trisulfone-2,4,6-trisulfone,	88(100)116(61)60(50)201(60)168(28)	1,3,5-Trisulfone-2,4,6-trisulfone, 6-(3-Methyl-Phenyl)-	300
4	1642	*	6-(3-Methyl-Phenyl) - ?	170(100)199(82)198(34)144(27)77(22)31(18)200(12)		
5	2002	*	C ₅ -Alkylquinoline	199(100)167(32)154(13)198(20)200(14)	108-Phenanthrene	580
			Phenanthrene			

TABLE A-92. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 35VI

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.16	--	Air	44(100)
2	.18	1-10	Dichloromethane	84(100)
3	.23	10-100	Chloroform	83(100)85(67)
4	.28	1-1	Benzene	78(100)
5	.34	1-10	Bromodichloromethane	83(100)85(63)129(8)127(6)
6	1.00	8	I.S.	75(100)110(30)

TABLE A-93. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 35VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum
1	0.13	-----	Air	44 (100)
2	0.20	1-10	Dichloromethane +	49 (100)
		1-10	Diethyl ether	59 (100) 45 (45) 74 (35)
3	0.26	10-100	Chloroform	83 (100) 85 (96)
4	0.30	10-100	Dichloroethane	62 (100) 44 (35) 96, 100
5	0.39	1-10	1,2-dichloropropane	63 (100) 62 (70) 76 (60) 41 (38) 65 (32) 97, 99, 101, 112, 114, 116
6	0.57	1-10	Toluene	91 (100) 92 (60)
7	0.72	1-10	1,1-di- <i>sec</i> -butoxy ethane	45 (100) 57 (60) 59 (30) 101 (30) 41 (28) 83 (8)
8	0.74	1-10	$\text{C}_{10}\text{H}_{22}\text{O}_2$ (T)	45 (100) 57 (70) 101 (32) 41 (30) 59 (25) 83 (8)
9	0.80	<1	Hydrocarbon M126	55 (100) 69 (70) 56 (65) 41 (60) 43 (28) 70 (22) 126 (9)
10	0.91	~1	C_7 Alkyl benzene	91 (100) 106 (60)
11	0.98	1-10	C_7 Alkyl benzene	91 (100) 106 (55)
12	1.00	~ 8	I S	75 (100) 77 (33)
13	1.19	1-10	Butyl ketone $\text{C}_9\text{H}_{18}\text{O}$	85 (100) 57 (75) 142, 41 (30) 58 (18) 127 (15)
14	1.21	~1	Unknown	43 (100) 84 (70) 69 (40) 85 (35) 99 (12)
15	1.22	1-10	C_9H_{10} eg Methyl styrene	117 (100) 118 (80) 115 (45) 91 (25) 103 (10)
16	1.24	1-10	C_9H_{10} eg Methyl styrene	117 (100) 118 (90) 115 (40) 91 (22) 103 (5)
17	1.29	<1	C_7 Alkyl benzene	105 (100) 120 (52)
18	1.32	1-10	C_9H_{10} eg Indene	115 (100) 116 (95) 117 (10) 89 (10)
19	1.52	<1	$\text{C}_{10}\text{H}_{10}$ eg cycloprop(2,3)indene or 4-ethyl benzene	130 (100) 129 (85) 128 (50) 115 (88) 102 (8)
20	1.53	1-10	$\text{C}_{10}\text{H}_{10}$ eg Divinyl benzene	130 (100) 115 (95) 129 (85) 128 (40)
21	1.63	~1	Unknown	95 (100) 137 (100) 123 (80) 43 (55) 109 (30) 81 (27) 91 (25) 41, 107, 121 (14)
22	1.76	1-10	Unknown	125 (100) 83 (70) 111 (45) 55 (38) 69 (30) 41 (23) 126 (20) 97 (10) 167 (8)
23	1.82	<1	Unknown	141 (100) 88 (87) 105 (50) 143 (35) 90 (30) 53 (28) 113 (15)

TABLE A-94. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 35E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic ions in Mass Spectrum	Most Reasonable Structure	R.I. ± 10
1	845	oo	Toluene	92 (100) 91 (95)	Benzene, methyl	843
2	848	oo	Dimethylpentane	57 (100) 43 (95) 58 (82) 114 (17) 99 (10) 86 (5) 71 (6)	2-Pentane	603
3	848	oo	Methylcyclohexane	83 (100) 55 (87) 98 (37)	3-Methyl-2-pentene	571
4	864	oo	C_6 -Ketone	57 (100) 39 (99) 85 (32) 101 (14) 114 (12)	2,4-Pentadiene	339
5	890	oo	Dimethylpentane	73 (100) 87 (48) 55 (65) 45 (39) 49 (26) 101 (8)	3-Pentene	879
6	916	oo	O-Xylene	91 (100) 106 (39) 77 (14) 51 (13) 45 (10) 43 (8)	Benzene, 1,2-dimethyl	894
7	921	oo	Xylene	91 (100) 106 (39) 67 (15) 51 (13) 55 (11)	Benzene, 1,2-dimethyl	443
8	931	oo	Dichloropropane	75 (100) 77 (32) 110 (30) 61 (27) 49 (22) 112 (18)		
9	942	oo	C_2 2, 9 Alkane + ?	43 (100) 45 (31) 101 (23) 87 (19)		
10	953	oo	C_6 -Alkylbenzene	57 (100) 105 (92) 85 (81) 120 (39) 142 (10)		
11	963	oo	Aldehyde $\text{C}_6\text{H}_{14}\text{O}$	43 (100) 86 (39) 69 (32) 118 (6) 117 (5)		
12	976	oo	Alkyl-alcohol	43 (100) 57 (35) 71 (49) 132 (14)		
13	980	oo	?	43 (100) 39 (51) 101 (28) 117 (10) 143 (3)		
14	987	oo	?	69 (100) 87 (38) 45 (32) 41 (32) 95 (2) 111 (2) 126 (2)		
15	995	oo	Decane + ?	57 (100) 43 (53) 85 (43) 86 (29) 45 (18)		
16	1008	oo				
17	1019	oo	C_7 -alkylbenzene	115 (100) 118 (93) 63 (19) 89 (18) 57 (15)		
18	1063	ooo	1-Hexyl-1-Phenylacetone	121 (100) 43 (99) 77 (27) 51 (23) 136 (6)	Benzene, 1-methyl	721
19	1100	oo	?	99 (100) 155 (58) 81 (54) 127 (45) 109 (33) 82 (32)		
20	1112	oo	Methylindene	115 (100) 130 (86) 129 (70) 83 (44) 126 (38) 117 (28)	1H-Indene, 3-methyl	323
21	1121	oo	Methylindene	115 (100) 130 (86) 129 (70) 128 (40) 119 (42)		
22	1164	oo	Naphthalene + ?	128 (100) 55 (65) 119 (42) 128 (16) 127 (13)		
23	1172	oo	Chloro-?	57 (100) 41 (38) 135 (15) 137 (5)		
24	1196	oo	C_6 -Alkylbenzene	91 (100) 119 (78) 134 (61) 43 (53) 162 (44) 83 (39)		
25	1240	ooo	Dihydroindene-1-one	104 (100) 132 (99) 78 (65) 51 (36)	1H-Indene-1-one	710
26	1265	oo	Methyltetrahydronaphthalene	131 (100) 146 (60) 117 (33) 103 (19) 91 (17) 43 (14) 51 (13) 167 (7)	Naphthalene, 1,2,3,4-tetrahydro-1-methyl	511
27	1274	oo	Methyltetrahydronaphthalene	131 (100) 146 (65) 103 (50) 77 (45) 57 (45)		
28	1307	oo	Dimethylbenzofuran	117 (100) 146 (80) 56 (50) 115 (42) 91 (25) 63 (22) 89 (17) 167 (11)		
29	1335	oo	Mixture of 28 + ?	87 (100) 118 (83) 90 (72) 146 (46) 154 (36)		
30	1347	oo	Mixture of 28 + ?	57 (100) 127 (61) 65 (38) 77 (30) 117 (11) 116 (10) 167 (7)		

TABLE A-94. (Continued)

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Match	
					Compound	ELI x 10 ³
31	1362	ee	Miscure ?	51(100) 55(27) 57(82) 54(50) 87(86) 114(12) 117(8)		
32	1376	ee	Miscure ?	43(100) 83(86) 125(88) 169(82) 91(76) 148(66) 181(56) 196(7)		
33	1381	ee	Miscure ? Ketone	57(100) 97(54) 59(32) 87(27) 181(12) 140(11) 196(4)		
34	1427	ee	Dichloro- ?	75(100) 79(54) 132(69) 111(26) 117(16) 109(16) 191(15) 193(5)		
35	1433	ee	Dichloro- ?	75(100) 141(87) 143(56) 111(45) 113(28) 77(30) 145(9)		
36	1447	ee	Dichloro- ?	79(100) 162(82) 119(50) 133(46) 91(36) 189(32) 191(30) 193(10)		
37	1862	ee	?	57(100) 56(69) 85(54) 135(40) 209(20) 211(7)		
38	1902	ee	?	56(100) 85(67) 135(50) 209(39) 93(36) 137(20) 211(15)		
39	1902	ee	?	75(100) 57(60) 111(40) 119(46) 155(41) 267(17) 265(12) 269(4)		
40	2047	ee	?	57(100) 75(68) 101(38) 97(26) 173(18) 247(9)		
41	2329	ee	?	57(100) 73(37) 101(22) 87(16) 113(14) 205(4)		

TABLE A-95. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 35E

GC Peak No.	Retention Time, min	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Mass Spectrometric Reference	
					Compound	Ref. No.
1	82.1	o	Dimethylbenzamide acid	73(100)74(25)77(81)81(51)99(20)115(4)	Benzoic acid, 3,3-Dimethyl-Methyl Ester	465
2	94.5	oo	?	43(100)85(72)102(53)109(17)115(13)		
3	83.7	oo	Acetoxybenzoic acid	73(100)71(74)63(74)35(44)59(21)87(20)113(16)128(4)	Benzoic acid, 5-(acetoxy)-Methyl Ester	332
4	86.8	o	Methylpentanoic acid	68(100)57(35)61(50)73(7)115(6)	Pentanoic acid, 2-Methyl, Methyl Ester	358
5	87.3	oo	C ≥ 6 Fatty acid	83(100)55(77)61(38)142(14)127(4)		
6	91.8	oo	C ≥ 6 Fatty acid	74(100)57(90)45(53)87(10)		
7	92.7	oo	C ≥ 6 Fatty acid	45(100)57(87)101(52)88(26)		
8	98.7	oo	1-Methyl-1-phenylethanol	43(100)121(63)77(18)51(13)136(2)	Benzoic methanol, o, o-Dimethyl	646
9	102.0	oo	Dimethylphenol	107(100)122(89)77(46)91(35)51(16)85(15)155(12)	Phenol, 2,4-Dimethyl	548
10	109.5	o	Allylthio-propionic acid ME	87(100)45(90)59(86)160(68)73(63)	Propionic acid, 3-(allylthio)-Methyl ester	437
11	110.5	oo	Methylbenzoic acid	119(100)118(64)91(79)45(35)150(27)	Benzoic acid, 2-Methyl, Methyl ester	448
12	113.5	oo	Methylbenzoic acid	119(100)91(63)150(31)65(26)	Benzoic acid, 2-Methyl, Methyl ester	451
13	116.4	ooo	Chloro?	57(100)87(28)135(18)89(6)137(5)		
14	118.8	oo	?	55(100)119(82)83(64)101(37)69(34)153(8)167(4)		
15	120.8	oo	Methyl-benzenepropanoic acid	119(100)91(65)77(16)103(12)178(10)51(6)65(4)		
16	123.5	oo	Hydroxy-methyl-benzoic acid	106(100)134(86)77(48)144(38)51(21)180(2)	Benzoic acid, 2-Hydroxy-4-Methyl-Methyl ester	443
17	127.6	oo	Ethyl-benzoic acid	136(100)103(40)77(39)162(32)56(15)163(4)	Benzoic acid, 4-Ethyl-Methyl ester	604
18	129.8	oo	Dimethylbenzoic acid	133(100)105(40)164(28)77(26)	Benzoic acid, 3,5-Dimethyl-Methyl ester	672
19	130.2	oo	Mixture?	172(100)97(97)113(89)157(82)125(71)79(72)59(68)		
20	131.8	ooo	Dimethyl-benzenepropanoic acid	119(100)91(58)135(16)77(14)65(15)165(4)192(7)		
21	132.9	oo	?	186(100)59(82)111(84)127(80)120(64)139(64)171(67)		
22	133.5	oo	?	59(100)77(56)75(55)171(44)186(55)		
23	136.2	oo	C ₁₃ -alkyl-phenyl propionic acid	119(100)91(80)77(16)78(10)51(7)206(2)		
24	141.0	oo	?	57(100)90(40)87(27)144(7)173(3)		
25	146.9	oo	Allylbenzoic acid	135(100)174(20)89(16)63(12)		
26	148.2	oo	Allylbenzoic acid	116(100)57(56)88(30)93(21)174(6)		
27	148.7	oo	?	87(100)85(92)55(90)59(60)184(10)		
28	170.2	oo	C ≥ 14 Fatty acid	87(100)102(91)		
29	187.2	oo	Bromo-?	135(100)75(68)99(66)117(19)267(6)245(5)		
30	246.5	oo	Phthalate	149(100)37(46)71(20)167(22)173(4)		

TABLE A-96. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 35E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Major Reasonable Monoamine Metabolite Compound	RI, $\times 10^3$
1	865	**	2-Propen-1-amine H ₂ O-2-Propenyl	110(100)41(86)68(83)96(30)82(30)127(19)	2-Propen-1-amine	315
2	917	**	2,4-Dichloroethanol	96(100)67(73)62(66)53(59)81(40)		
3	924	**	1-Butanol 4-Butoxy	57(100)41(67)73(21)87(8)134(3)		
4	965	**	?	121(100)43(60)77(21)139(12)91(12)105(6)		
5	1030	*	Dimethylamine	120(100)106(98)121(97)		
6	1040	**	?	156(100)132(55)104(44)79(43)127(42)141(40)		
7	1121	**	?	57(100)41(66)87(31)116(11)117(8)		
8	1136	**	Alkyl ketone	125(100)43(66)83(62)181(43)69(41)97(34)139(22)196(8)		
9	1166	**	Dihydroindene-1,2-Diol + ?	106(100)103(99)132(56)131(42)77(43)91(38)150(20)	1H-Indene-1,2-Diol	792
10	1235	**	1H Indene-1,2-Diol-2,3-Dihydro + ?	106(100)77(52)112(48)131(38)91(43)150(16)	1H-Indene-1,2-Diol	762
			* Neutral compounds were so concentrated that they were also extracted into basic fraction			

TABLE A-97. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 36VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.10	----	air	44(100)
2	0.14	1-10	Dichloromethane	49(100)
3	0.20	10-100	Chloroform	83(100)
4	0.24	1-10	1,1,1-Trichloroethane	97(100)99(70)81(45)117,119,121
5	0.34	10-100	Bromodichloromethane	83(100)85(65)47(23)127,129,131
6	0.58	1-10	Dibromochloromethane	129(100)127(60)131(30)79,81,206,208,210
7	1.00	- 8	I S	75(100)110(60)

TABLE A-98. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 37VI-a

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44 (100)
2	0.16	<1	Acetone	43 (100) 58 (28)
3	0.16	<1	Diethylether	45 (100) 59 (97) 74 (55)
4	0.17	10-100	Dichloromethane	69 (100) 84 (77)
5	0.25	<1	Tetrahydrofuran	42 (100) 41 (67) 39 (40) 72 (32) 71 (30)
6	0.26	<1	1,1,1-Trichloroethane	97 (100) 99 (60) 81 (51)
7	0.29	<1	Benzene	78 (100)
8	0.34	<1	Dichloropropane	63 (100) 62 (75) 41 (60) 39 (42) 65 (32) 76 (30)
9	0.36	<1	Trichloroethylene	95 (100) 110, 132 (90)
10	1.00	-(8)	IS	75 (100) 77 (33)

TABLE A-99. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 37VI-b

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.086	--	Air	44 (100)
2	0.12	<1	Acetone	43 (100) 58 (30)
3	0.12	<1	Diethylether	59 (100) 74 (80) 45 (65)
4	0.13	1-10	Dichloromethane	84 (100) 49 (90)
5	0.22	<1	Tetrahydrofuran	42 (100) 41 (65) 72 (33) 36 (31) 71 (29)
6	0.23	<1	1,1,1-Trichloroethane	97 (100) 61 (70) 99 (62) 117 (12)
7	0.25	<1	Benzene	78 (100)
8	0.31	<1	Dichloropropane	63 (100) 62 (72) 41 (55)
9	1.00	-(8)	IS	75 (100)

TABLE A-100. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 37VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic ions in Mass Spectrum
1	0.13	---	air	44(100)
2	0.14	<1	Butene	41(100)36(85)
3	0.18	<1 ea	Dimethyl sulfide + Dichloromethylene	47(100)81(85)65(70)81(50)46(45)96(8)98(6)
4	0.18	1-10	Dichloromethane	49(100)
5	0.26	<1	Tetrahydrofuran	42(100)41(52)71,72(40)
6	0.50	<1	Toluene	91(100)92(60)
7	---	<1	C ₂ -Methyl benzene	91(100)106(38)
8	---	<1	C ₂ -Methyl benzene	91(100)
9	---	---	I S	75(100)

TABLE A-101. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 38VI

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44(100)
2	0.13	1-10	Dimethyl ether (T)	45(100)46(50)
3	0.13	~ 1	Butene	41(100)39(70)36(30)
4	0.16	1-10	n-pentane	43(100)42(65)41(50)39(20)37(9)72(5)
5	0.16	each 1-10	Diethyl ether + dichloroethylene	45(100)59(89)74(40)96(30)98(23)
6	0.16	20-30	Dichloromethane	69,51,86,86(100) (Sat'd.)
7	0.21	1-10	Dichloroethylene	81(100)96(70)90(42)
8	0.22	each 10-20	Chloroform + alkane	61(100)57(68)48(82)83(75)85(48)
9	0.24	~ 1	Tetrahydrofuran	42(100)71,72(28)
10	0.25	1-10	Dichloroethane	62(100)64(33)98(8)100(6)
11	0.26	1-10	1,1,1-Trichloroethane	97(100)99(67)61(45)117,119(18)
12	0.29	<1	Benzene	78(100)
13	0.29	<1	Carbon tetrachloride	117,119(100)67(50)35(40)82(15)
14	0.36	10-20	Trichloroethylene	95(100)130(85)132(83)97(65)
15	0.66	1-10	1,1,2,2-Tetrachloroethane	129(100)131(96)166(90)164(80)
16	0.68	1-10	Di-butoxyethane (T)	65(100)57(70)41(36)101(30)
17	0.71	1-10	Di-butoxyethane (T)	65(100)57(75)41(36)101(28)
18	1.00	-(8)	IS	75(100)77(13)
19	1.32	1-10	Dichlorobenzene	75(100)146,50(89)111(80)148(60)

TABLE A-102. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 38VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44(100)
2	0.15	>100	Acetone	43(100) 58(30)
3	0.17	1-10	Dichloroethylene + Ethyl mercaptan	62(100) 47(88) 61(82) 65(55) 46(38) 96(30) 98(20) 100(3)
4	0.18	10-100	Dichloromethane	49(100)
5	0.26	10-100	Chloroform	83(100)
6	0.29	1-10	1,2-Dichloroethane	62(100) 84(33) 49(20) 98(10) 100, 102
7	0.31	>10	1,1,1-Trichloroethane	97(100) 99(60) 61(50) 117, 119, 121
8	0.33	1-10	Benzene	78(100)
9	0.41	1-10	Trichloroethylene	95(100) 132(98) 130(96) 97(65) 60(43) 134(30)
10	0.51	1-10	Methylisobutyl ketone	43(100) 58(42) 57, 85(25) 100(20)
11	0.57	1-10	Toluene	91(100) 92(60)
12	0.70	1-10	1,1,2,2-Tetrachloroethene	166(100) 164(80) 129, 131(73) 166(50) 94(50)
13	0.92	1-10	C ₂ -Alkyl benzene	91(100) 106(60)
14	0.98	1-10	C ₂ -Alkyl benzene	91(100) 106(63)
15	1.00	--	I.S.	75(100)
16	1.24	1-10	C ₃ -Alkyl benzene	91(100) 106(60)
17	1.30	1-10	Dichlorobenzene	146(100) 148(60) 111(20) 150(10)

TABLE A-103. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 39VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.10	--	Air	44(100)
2	0.10	>>100	Dimethylether	45(100)45(98)47(40)43(14)
3	0.12	10-100	Acetone	43(100)
4	0.15	10-100	Dichloromethane	49(100)
5	0.19	1-10	Chloroform	83(100)
6	0.23	<1	1,2-Dichloroethane	62(100)64(33)49(30)96,100
7	0.24	<1	1,1,1-Trichloroethane	97(100)99(67)81(55)78(38)117,119,121(8)
8	0.27	<1	Benzene	78(100)
9	0.35	<1	Trichloroethylene	95(100)130,132(90)97(60)80(38)134(33)
10	0.55	<1	Toluene	91(100)
11	0.70	<1	1,1,1,2-Tetrachloroethane	166(100)139,131(88)164(83)168(50)94(45)
12	0.93	<1	C ₂ -Alkyl benzene	91(100)106(30)
13	0.98	<1	C ₂ -Alkyl benzene	91(100)106(42)
14	1.06	<1	C ₂ -Alkyl benzene	91(100)106(45)
15	1.30	<1	C ₂ -Alkyl benzene	91(100)106(35)
16	1.31	<1	C ₃ -Alkyl benzene	105(100)120(28)
17	1.39	<1	C ₃ -Alkyl benzene	105(100)120(50)
18	1.46	1-10	Dichlorobenzene	146(100)148(67)111(33)113,150(10)

TABLE A-104. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 40VI

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.14	---	Air	44(100)
2	0.17	1-10	Acetone + C_5H_{10} ag	43(100)55(50)58(32)70(20)
3	0.18	1-10	2-Methyl-2-butene	45(100)44(68)59(50)76(10)
4	0.19	1-10	2-chloropropene + 2-butanol (T)	49(100)
5	0.20	1-10	Dichloromethane	43(100)41(72)72(55)
6	0.21	<1	Isobutyraldehyde (T)	43(100)44(65)45(33)67(6)68(3)
7	0.21	<1	Unknown	41(100)70(70)42(28)
8	0.23	<1	2-Methylpropenal (T)	43,44(100)41(61)57(22)72(38)
9	0.23	<1	Butyraldehyde	43(100)72(18)57(10)
10	0.25	1-10	Methyl ethyl ketone	83(100)85(67)
11	0.28	1-10	Chloroform	62(100)64(31)49(25)98(8)100(6)
12	0.29	<1	1,2-Dichloroethane	97(100)99(65)61(62)117,119(10)
13	0.31	<1	1,1,1-Trichloroethane	43(100)41(15)86(12)
14	0.32	<1	3-Methyl-2-butanone	78(100)41(60)57(60)58(50)
15	0.38	10-100	Benzene + Unknown	63(100)62(70)41(40)76(40) 97,99,112,114
16	0.40	<1	1,2-Dichloropropene	95(100)130,132(90)97(60)60(50)134(30)
17	0.70	<1	Trichloroethylene	166(100)164,129,131(90)94(60)168(58)
18	0.80	<1	1,1,2,2-Tetrachloroethane	112(100)77(75)114(35)50,51(30)
19	0.97	<1	Chlorobenzene	91(100)106(40)
20	1.00	---	C_7 Alkyl benzene	75(100)
			I, S,	

TABLE A-105. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 40VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	---		Air	
2	---		Dichloromethane	49(100)
3	---	>100	Chloroform	
4	---	10-100	C ₂ Alkyl benzene	
5	---	10-100	C ₂ Alkyl benzene	
6	---	10-100	C ₂ Alkyl benzene	
7	---	>100	Unknown (Saturated Spectrum)	
8	---	10-100	C ₂ Alkyl benzene	
9	---	>100	Unknown (Saturated Spectrum)	

TABLE A-106. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 401

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Typical Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Monomer Molecule	Ref. #
1	844	oo	C ₂ - 9 Alkane	43 (100) 166 (55) 165 (43) 129 (40) 131 (40) 133 (12) 168 (26) 170 (6)		
2	859	oo	Toluene	92 (100) 91 (85) 165 (64) 163 (40) 51 (33) 93 (18)		
3	870	oo	Ethylbenzene	91 (100) 106 (28) 51 (12) 65 (12) 77 (10)	Benzene, ethyl	755
4	876	oo	o-Xylene	91 (100) 106 (53) 105 (25) 77 (17) 65 (11) 107 (5)	Benzene, 1,2-dimethyl	632
5	891	oo	p-Xylene	91 (100) 106 (38) 77 (13) 51 (12) 65 (9)		
6	907	oo	Benzene	43 (100) 37 (85) 41 (56) 85 (28) 71 (21) 99 (7) 128 (3)		
7	951	oo	C ₁ -Alkylbenzene	105 (100) 120 (26) 77 (19) 91 (15) 79 (16) 65 (10)		
8	957	oo	C ₂ -Alkylbenzene	105 (100) 120 (46) 77 (15) 91 (12) 57 (9) 51 (8)	Benzene, 1-ethyl-3-methyl	670
9	966	oo	C ₃ -Alkylbenzene	105 (100) 43 (32) 57 (31) 120 (29)	Benzene, (1-methyl ethyl)	361
10	982	oo	C ₄ -Alkylbenzene	105 (100) 120 (35) 77 (15) 51 (10) 91 (12)		
11	1005	oo	Decane	57 (100) 43 (90) 41 (69) 71 (40) 85 (26) 99 (7) 142 (6)	Hexane	893
12	1008	oo	C ₅ -Alkylbenzene	105 (100) 120 (36) 77 (17) 57 (13) 79 (12) 91 (13)	Benzene, 1-ethyl-3-methyl	603
13	1017	oo	Heptylbenzene	117 (100) 118 (55) 115 (35) 91 (20) 63 (16) 119 (6)	Benzene, 1-ethyl-2-methyl	749
14	1037	oo	C ₆ -Alkylbenzene	105 (100) 77 (34) 57 (25) 41 (18) 43 (17) 134 (9)		
15	1053	oo	C ₇ -Alkylbenzene	119 (100) 134 (23) 91 (13) 77 (12) 51 (5)		
16	1063	oo	C ₈ -Alkylbenzene	119 (100) 117 (38) 91 (31) 57 (25) 43 (20) 71 (16) 134 (26)		
17	1067	oo	C ₉ -Alkylbenzene	119 (100) 43 (70) 57 (35) 91 (32) 117 (30) 134 (26)		
18	1103	oo	Dodecane	57 (100) 43 (86) 71 (46) 85 (26) 156 (2)		
19	1119	oo	C ₁₀ -Alkylbenzene	117 (100) 131 (34) 132 (33) 91 (29) 77 (11) 51 (9) 64 (7) 146 (8)		
20	1128	oo	C ₁₁ -Alkylbenzene	117 (100) 115 (79) 132 (29) 91 (26) 51 (12) 77 (13) 146 (2)		
21	1157	oo	Heptadecane	128 (100) 43 (26) 57 (23) 71 (18) 127 (17) 129 (10)		

TABLE A-107. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 40E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Numerous Observed Ion	$\frac{M}{z}$
1	867	oo	Ethylbenzene	91 (100) 106 (28) 51 (13) 65 (12) 77 (10)	Benzene, ethyl	760
2	873	ooo	O-Xylene	91 (100) 106 (43) 77 (13) 51 (10) 65 (8) 63 (6)	Benzene, 1,2-dimethyl	728
3	880	ooo	P-Xylene	91 (100) 106 (78)	Benzene, 1,4-dimethyl	480
4	999	oo	Chlorocyclohexanol	57 (100) 86 (24) 86 (10) 96 (8) 134 (3) 135 (0.6)	Cyclohexanol, 4-chloro, trans	561
5	1034	oo	Dichlorocyclohexane	81 (100) 80 (38) 78 (21) 135 (1) 134 (0.5)	Cyclohexane, 1,2-dichloro	627
6	1068	oo	Bromocyclohexanol	81 (100) 57 (66) 99 (26) 132 (3) 134 (3) 180 (1) 178 (1)	Cyclohexanol, 2-bromo	536
7	1111	oo	Bromochlorocyclohexane	81 (100) 79 (17) 53 (13) 117 (6) 119 (2)	Cyclohexane, 1-bromo-2-chloro, cis	645
8	1551	oo	Diethyl phthalate	149 (100) 150 (12) 105 (9) 65 (8) 177 (17) 222 (0.6)	1,2-benzenedicarboxylic acid diethyl ester	630
9	1902	oo	Nonadecane	57 (100) 43 (76) 71 (71) 85 (48) 99 (13) 113 (9) 127 (5)	Eicosane	722
10	1979	oo	Sub. Cyclohexane carboxylic acid methyl ester	134 (100) 107 (37) 37 (36) 79 (24) 167 (19) 186 (18) 234 (7)	1-cyclohexene-1-carboxylic acid, 2-(1,3-dimethyl-3-oxobutyl)-methyl ester	640
11	2011		Eicosane			
12	2297	oo	Bis(2-ethylhexyl) malonate	149 (100) 91 (71) 65 (18) 150 (11) 206 (19) 238 (2)		
13	2497	oo	Perfluorooctane			
14	2702	oo	Perfluorodecane			

TABLE A-108. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 40E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Terminal Identification	Characteristic ions in Mass Spectrum	Most Reasonable Saturated Alcohol	Ref. #
1	1109	e	C $\geq$ 8 Fatty acid	74(100)87(66)183(4)185(3)214(1)	Undecanoic acid, 10-methyl, methyl ester	518
2	1707	e	Tetradecanoic acid	74(100)87(68)143(36)55(26)143(12)157(4)213(2)	Tetradecanoic acid, methyl ester	872
3	1910	ee	Hexadecanoic acid	74(66)87(68)227(2)270(1)		
4	1979	ee	C $\geq$ 16 Fatty acid	74(100)87(73)143(20)185(7)241(3)284(2)		
5	2008	e	C $\geq$ 17 Fatty acid	74(100)87(74)143(16)241(3)		
6	2051	e	C $\geq$ 18 Fatty acid	74(100)87(75)143(20)	Heptadecanoic acid, 16-methyl, methyl ester	490
7	2073	e	C $\geq$ 18 Fatty acid	74(100)87(80)		
8	2110	ee	Octadecanoic acid	41(100)74(99)87(75)143(17)196(5)255(3)298(1)	Heptadecanoic acid, 16-methyl, methyl ester	395
9	2190		C $\geq$ 18 Fatty acid	74(100)87(18)143(38)143(22)299(2)	Heptadecanoic acid, 15-methyl, methyl ester	643
10	2302	ee	C $\geq$ 20 Fatty acid + Phthalate	149(100)91(73)237(43)197(37)195(30)312(13)		
11	2314	ee	C $\geq$ 20 Fatty acid	237(100)74(80)87(66)128(28)143(27)182(16)297(8)312(8)		
12	2475	ee	C $\geq$ 21 Fatty acid	74(100)87(33)		
13	2517	ee	C $\geq$ 22 Fatty acid	74(100)87(77)143(21)255(1.5)354(1.5)		
14	2677	e	C $\geq$ 23 Fatty acid	74(100)87(81)143(17)		
15	2715	e	C $\geq$ 24 Fatty acid	74(100)87(87)143(21)		

TABLE A-109. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 41VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	--	Air	44(100)
2	0.13	>100	Dimethyl ether (T)	43-45(100) (Sat'd spectrum)
3	0.17	>100	Acetone	43(100)58(30)
4	0.18	>100	Dichloroethane	49(100)
5	0.24	1-10	Chloroform	83(100)
6	0.28	1-10	1,1,1-Trichloroethane	97(100)99(67)61(40)119(12)117(10)121(4)
7	0.91	1-10	C ₂ -Alkyl benzene	91(100)106(60)
8	0.98	1-10	C ₂ -Alkyl benzene	91(100)106(40)
9	1.00	--	I.S.	75(100)77(33)

TABLE A-110. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 42VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.14	--	Air	44(100)
2	0.18	1-10	1,1-Dichloroethylene	61(100)96(65)98(40)63(33)
3	0.19	1-10	Dichloromethane	84(100)49(95)
4	0.24	1-10	Methylethyl ketone	43(100)72(20)57(6)
5	0.26	1-10	Chloroform	83(100)
6	0.28	<1	2-Chloro-2-butene	55(100)90(35)54(33)53(25)41(18)50(13)92(11)
7	0.28	<1	Tetrahydrofuran	42(100)41(55)71, 72(40)
8	0.29	<1	1,2-Dichloroethane	62(100)64(33)49(29)98(10)10(5)
9	0.30	1-10	1,1,1-Trichloroethane	97(100)99(70)61(52)117, 119(8)
10	0.38	1-10	1,2-Dichloropropane	63(100)62(75)41(55)76(45)65(30)
11	0.40	10-100	Bromodichloromethane	83(100)85(65)129(10)127(8)131(2)
12	0.57	<1	Toluene	91(100)92(56)
13	0.61	10-100	Dibromochloromethane	129(100)127(82)79, 81, 131(25)
14	0.90	1-10	Bromoform	173(100)171(60)175(48)79, 81(35)252, 254(5)
15	1.00	--	I.S.	75(100)

TABLE A-111. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 43VI

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	---	air	44(100)
2	0.18	10-100	Dichloromethane	49(100)
3	0.52	<1	methyl isobutyl ketone	43(100)58(30)85(16)100(9) (also seen in previous run)
4	0.81	---	Chlorobenzene	112(100)77(72)50,51,114(32)
5	0.98	---	C ₃ alkyl benzene	91(100)106(40)
6	1.00	---	1.5	75(100)

TABLE A-112. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 43VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	---	Air	
2	0.18	1-10	Dichloromethane	49(100)
3	0.28	1-10	1,1,1-trichloroethane	97(100)99(47)61(50)
4	0.31	1-10	Benzene	78(100)
5	0.49	1-10	Methyl isobutyl ketone	58(100)43(99)57(57)41(46)85(43)100(30)
6	0.55	<1	Toluene	91(100)92(53)
7	0.59	1-10	n-Butyl acetate	43(100)56(25)73(12)
8	0.91	1-10	C ₂ -Alkyl benzene	91(100)106(47)
9	0.97	1-10	C ₂ -Alkyl benzene	91(100)106(45)
10	1.00	---	1.5.	75(100)110(35)

TABLE A-113. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 43I

GC Peak No.	Retention Index	Amount, μ g/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Structure Match	R.I. $\times 10^3$
1	844	++	Dichloro C_8 -alkane	41(100)55(83)90(63)77(43)92(17)126(4)126(3)	Compound	
2	855	+	Chlorohexane	91(100)55(80)93(33)41(63)		
3	915	++	Chloromethylbutane	55(100)69(68)68(56)41(30)91(31)93(9)104(4)104(2)	Hexane, 1-Chloro-	646
4	1010	++	?	89(100)41(52)82(26)67(20)90(8)105(4)118(2)	1-Butene, 2-(Chloromethyl)-	358
5	1056	+	Chlorosthenylbenzene	89(100)125(95)55(70)83(41)91(33)127(60)138(4)140(2)		
6	1030	++	Benzene sulfonamide N,4-Dimethyl	91(100)65(29)121(23)150(26)92(20)185(27)186(3)		
7	2110	+	C $\geq$ 18 Fatty Acid	74(100)87(80)143(23)298(3)	Benzenesulfonamide, N,4-Dimethyl	595
					Heptadecanoic Acid, 16-Methyl-, Methyl Ester	540
8	2321	+	C $\geq$ 20 Fatty Acid	87(100)55(100)97(66)197(83)200(23)229(8)	Octadecanoic Acid, 12-Hydroxy-, Methyl Ester	601

TABLE A-114. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 43E

GC Peak No.	Retention Index	Amount, μ g/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Structure Match	R.I. $\times 10^3$
1	976	+++	Phenol	94(100)84(48)55(26)95(4)	Compound	
2	1042	++	Methylalano	108(100)107(96)79(46)77(44)		
3	1064	+++	Methylalano	41(100)107(80)77(25)79(10)109(5)		
4	1137	++	Dimethylphenol	107(100)122(76)121(40)77(36)79(22)91(27)	Phenol, 3,4-Dimethyl	532
5	1162	++	Dimethylphenol	107(100)122(82)77(33)79(21)91(22)	Phenol, 2,5-Dimethyl	542
6	1309	+	C $\geq$ 10 Fatty acid	74(100)87(67)143(13)171(9)	Decanoic acid, 8-Methyl-, Methyl ester	457
7	1708	+	C $\geq$ 12 Fatty acid	74(100)87(76)143(20)199(12)	Undecanoic acid, 11-Bromo, Methyl ester	489
8	2080	+	C $\geq$ 17 Fatty acid	74(57)87(35)264(6)	10-Hydroxycanoic acid, methyl ester	478
9	2110	+	C $\geq$ 18 Fatty acid	74(100)87(70)143(13)199(6)255(4)	Tricosanoic acid, methyl ester	354

TABLE A-115. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 44VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.14	—	Air	44(100)
2	0.18	10-100	Acetone	43(100)58(30)
3	0.19	10-100	Dichloromethane	84(100)49(73)86(62)
4	0.23	1-10	Methyl ethyl ketone	43(100)72(20)
5	0.32	1-10	Benzene	78(100)
6	0.57	1-10	Toluene	91(100)92(55)
7	1.00	~8	1,5.	75(100)77(33)

TABLE A-116. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 44E

GC Peak No.	Retention Index	Amount, μg^1	Tentative Identification	Characteristic Ions in Mass Spectrum	Mass Resolvable Elements Match	
					Compound	R.I. at 10 ³
1	970	ooo	Phenol	94 (100) 44 (46) 65 (25) 95 (7) 95 (4)	Phenol, 2-Methyl	370
2	1038	ooo	Methylphenol	108 (100) 107 (92) 79 (38) 77 (37) 51 (15) 65 (9) 90 (8) 89 (14) 91 (7)		
3	1062	ooo	C ₂ -Alkylphenol	107 (100) 106 (75) 77 (38) 79 (34) 122 (10) 51 (13) 55 (11)		
5	1125	oo	C ₂ -Alkylphenol	107 (100) 122 (42) 77 (33) 79 (17) 51 (9) 65 (8) 65 (7) 123 (4)		
6	1131	ooo	C ₂ -Alkylphenol	107 (100) 122 (81) 121 (47) 77 (28) 91 (25) 79 (19) 51 (9) 123 (6)		
7	1154	ooo	C ₂ -Alkylphenol	107 (100) 122 (40) 77 (22) 91 (9) 79 (7) 65 (6) 51 (7) 123 (7) 138 (2)		
8	1182	oo	C ₂ -Alkylphenol	107 (100) 122 (92) 121 (71) 77 (42) 91 (29) 136 (5)		
9	1212	oo	C ₂ -Alkylphenol	121 (100) 136 (41) 91 (31) 77 (26) 167 (15) 65 (8) 51 (8)	Phenol, 3-Ethyl-5-Methyl	473
10	1222	oo	C ₂ -Alkylphenol	121 (100) 136 (27) 91 (17) 77 (15) 65 (5) 51 (4) 103 (4) 107 (4)		
11	1245	oo	C ₂ -Alkylphenol	121 (100) 136 (61) 107 (41) 77 (27) 91 (26) 65 (7) 55 (5)		
12	1253	oo	C ₂ -Alkylphenol	121 (100) 136 (67) 91 (38) 77 (26) 107 (14) 79 (10) 65 (8) 53 (8)		
13	1268	o	C ₂ -Alkylphenol	121 (100) 136 (35) 91 (23) 77 (20) 107 (15) 65 (8) 51 (7)		
14	1321	oo	C ₂ -Alkylphenol	133 (100) 134 (90) 135 (59) 105 (40) 91 (43) 77 (46) 51 (21) 65 (17)		
15	1330	oo	C ₂ -Alkylphenol	133 (100) 136 (53) 135 (27) 105 (33) 77 (27) 91 (20) 150 (20) 51 (20)		
16	1343	o	Methylallylphenol	133 (100) 107 (90) 148 (40) 77 (35) 63 (16) 51 (16) 162 (5)	Phenol, 2-(2-methyl-2-propenyl)	493
17	1370	oo	C ₂ -Alkylphenol + ?	133 (100) 148 (34) 105 (26) 77 (13) 91 (9) 51 (7) 63 (7)		
18	1389	o	C ₂ -Alkylphenol	133 (100) 148 (57) 105 (22) 91 (22) 77 (17) 63 (12) 149 (12)		
19	1424	oo	C ₂ -Alkylphenol + ?	133 (100) 147 (61) 148 (55) 91 (19) 105 (18) 77 (14) 51 (10) 162 (7) 166 (1)		
4	1083	oo	Benzoic Acid	105 (100) 77 (60) 136 (40) 51 (28)		

TABLE A-117. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 45VI

GC Peak No.	Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44(100)
2	0.16	<1	Diethylether	45(100)59(95)74(50)
3	0.16	>10	Dichloromethane	69(100)84(37)51(28)
4	0.32	<1	Chloroform	83(100)85(67)
5	0.24	<1	Tetrahydrofuran	42(100)41(77)71,72(33)
6	0.26	<1	1,1,1-Trichloroethane	97(100)99(65)
7	0.28	<1	Benzene	78(100)
8	0.35	<1	Trichloroethylene	95(100)132(80)130(78)
9	0.67	>10	1,1,2,2-Tetrachloroethane	166(100)129(90)131(85)
10	1.00	-(8)	IS	75(100)77(33)

TABLE A-118. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 45VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Retention Identification	Characteristic Ion in Mass Spectrum
1	0.11	---	Alk	44 (100)
2	0.12	10-100	Butene	56 (100) 41 (98)
3	0.17	10-100	Chloromethyl propane	72 (100) 55 (82) 43 (78) 90 (49) 95 (12) 72 + unknown
4	0.22	>100	Chloromethyl propane	90 (100) 54 (95) 55 (90)
5	0.32	10-100	Benzene	78 (100)
6	0.36	>100	Dibromomethane	93 (100) 174 (90) 95 (85) 172 (50) 79, 81 (25)
6	0.36	>100	Dibromomethane	93 (100) 174 (90) 95 (85) 172 (50) 79, 81 (25)
7	0.49	10-100	Unknown	93 (100) 91 (72) 77 (58) 108 (33)
8	0.51	10-100	$\text{C}_8\text{H}_8\text{Cl}_2$ 1,3-dichloro-2-methyl propane	77 (100) 55 (80) 79 (70) 41 (60) 91 (35) 75 (30) 49 (25) 76 (20) 93 (10) 111 (8) 113 (5)
9	0.56	>100	Toluene	91 (100) 92 (65)
10	0.60	>100	Unknown	65 (100) 51 (60) 63 (58) 50 (42) 62 (25) 89 (25) 93 (20) 45 (20)
11	0.67	1-10	Unknown	64 (100) 55 (90) 90 (72) 65 (50) 75 (28)
12	0.69	1-10	Unknown	55 (100) 67 (70) 95 (60) 68 (60) 53 (28) 41 (25) 81 (15)
13	0.69	1-10	Unknown	55 (100) 41 (85) 77 (80) 54 (65) 76 (40) 90 (28)
14	0.71	1-10	C_8H_{14} 2,4-hexadiene	95 (100) 67 (80) 55 (34) 45 (30) 110 (28)
15	0.72	1-10	C_8H_{14} + Unknown	95 (100) 93 (80) 91 (68) 67 (60) 77 (48) 55 (42) 108 (40) 110 (26)
16	0.75	1-10	C_8H_{14} + Tetrachloroethane	95 (100) 67 (40) 110 (28) 93 (25) Small 129, 131, 164, 166, 168
17	0.82	>100	$\text{C}_8\text{H}_8\text{Cl}_2$	89 (100) 53 (98) 124 (50) 91 (48) 126 (33) 50 (30)
18	0.86	>100	1,3-dichloro-2-methylpropane	88 (100) 89 (65) 53 (40) 90 (50) 49 (38)
19	0.93	10-100	C_8H_{12}	93 (100) 91 (90) 77 (60) 108 (60) 79 (48)
20	0.94	10-100	Unknown	55 (100) 46 (70) 116 (70) 87 (50)
21	0.95	10-100	C_7 Alkyl benzene	91 (100) 106 (33)
22	0.96	10-100	Unknown	93 (100) 91 (55) 108 (50) 77 (50) 55 (40) 171, 173, 175
23	0.98	10-100	C_8H_{10}	106 (100) 105 (60) 91 (43) 77 (28) 56 (22)
24	0.99	10-100	Unknown	101 (100) 55 (64) 73 (53) 43 (35)
25	1.01	10-100	C_8H_{14}	67 (100) 95 (95) 110 (90) 55 (38) 41 (30)
26	1.02	10-100	Unknown	77 (100) 79 (30) 70 (28) 41 (26) 125 (12) 127 (8)
27	1.04	10-100	C_7 Alkyl benzene	91 (100) 106 (40)
28	1.06	10-100	Unknown	77 (100) 93 (100) 91 (95) 108 (55) 75 (50) 126 (8)
29	1.09	10-100	Unknown	53 (100) 89 (70) 88 (72)

TABLE A-118. (Continued)

QC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
30	1.10	10-100	Diethyl disulfide	122(100)66(82)94(50)124(8)
31	1.17	>100	Unknown	113(100)75(100)111(95)58(64)49(54)124(15)
32	1.32	10-100	Unknown	109(100)67(60)41(24)77(22)91(21)
33	1.35	10-100	Unknown	109(100)55(98)53(72)67(65)142(6)
34	1.52	10-100	C ₈ alkyl benzene	133(100)105(70)148(55)77(22)
35	1.54	10-100	1-methene C ₁₁ H ₁₂ M146 2,3-dihydro-2,3-dimethyl	131(100)91,119,146(40)
36	1.56	10-100	C ₁₁ H ₁₄ , eg methyl butenyl benzene	131(100)91(42)146(40)105(30)77(22)
37	1.58	10-100	C ₁₁ H ₁₄	131(100)91(53)146(50)105(30)
38	1.61	>100	Unknown	121(100)93(95)97(90)65(90)115(60)109(50)198(30)
39	1.65	10-100	C ₁₁ H ₁₄ , eg 1,1-dimethyl-2-propenyl benzene	131(100)91(62)146(50)115(38)
40	1.66	10-100	Unknown	55(100)91(50)90(25)93(23)143(18)158(8)
41	1.67	10-100	2,3-di hydro-4,7-dimethyl 1-methene C ₁₁ H ₁₄ M146	131(100)146(70)91(42)115(30)
42	1.73	10-100	4-(2-butenyl)-1,2-dimethyl benzene C ₁₂ H ₁₆ M160	145(100)91(88)160(40)55(55)
43	1.95	10-100	1-(2-butenyl)-2,3-dimethyl benzene C ₁₂ H ₁₆ M160	145(100)105(40)125(30)124(30) (no 160)

TABLE A-119. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 45E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Typical Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Benzene Derivative Compound	EL, $\times 10^3$
1	873	***	$\text{C}_8\text{H}_{10}\text{Cl}_2$	89 (100) 33 (99) 91 (35) 124 (31) 126 (20)		
2	877	ee	$\text{C}_8\text{H}_{10}\text{Cl}_2$ Dichlorobutene	88 (100) 89 (89) 33 (94) 90 (38) 124 (14) 126 (9) 128 (1)		
3	883	ee	Methylpentanone	61 (100) 85 (55) 63 (55) 65 (18) 57 (16)	2-Pentanone, 4-methyl	458
4	891	ee	Xylene + ?	55 (80) 73 (78) 91 (56) 106 (21)		
5	905	ee	2-Propenal-1 (2-furalyl)	71 (100) 66 (76) 122 (65) 63 (50) 96 (44) 124 (6)		
6	933	***	Chloro-alkene	111 (100) 75 (81) 113 (66) 77 (25) 89 (23) 124 (9) 126 (6)		
7	950	ee	?	43 (100) 99 (76) 55 (58) 70 (35) 100 (4)		
8	1003	ee	Chloro-alkene	41 (100) 43 (40) 85 (30) 57 (16) 87 (5) 99 (0-6) 97 (0-4)		
9	1037	ee	Acetophenone	105 (100) 77 (88) 51 (36) 120 (24)	Ethanol, 1-phenyl	719
10	1049	ee	1-Methyl-1-phenylethanol	79 (100) 107 (74) 77 (57) 122 (22) 51 (24)	Benzene methanol, 4-methyl	657
11	1095	***	C_5 -alkylbenzene	125 (100) 105 (70) 148 (37) 77 (19) 91 (20) 51 (19) 43 (12)	Benzene, 1-methyl-3-(1-methyl ethyl)	440
12	1115	ee	?	61 (100) 154 (70) 94 (33) 122 (16) 156 (8)		
13	1143	***	Mixture + Benzene, 1,1'-oxybis(1-methyl)	97 (99) 121 (92) 65 (94) 93 (93) 81 (47) 170 (17) 198 (100) 199 (8)		
14	1176	***	Ethanol, 1-(2-butoxyethoxy)	45 (100) 57 (80) 75 (17) 87 (10) 89 (8) 132 (1)	Ethanol, 1-(2-butoxy ethoxy)	617
15	1194	ee	3(2H)-Benzofuranone, dimethyl	94 (100) 162 (56) 76 (38) 104 (36) 43 (33) 121 (28) 147 (22)		
16	1208	ee	?	75 (100) 111 (65) 99 (48) 157 (42) 50 (38) 127 (22) 159 (14)		
17	1231	ee	Benzoic acid, 2-propenyl ester	105 (100) 77 (42) 51 (20) 117 (5) 162 (2)	Benzoic acid, 2-propenyl ester	382
18	1255	ee	3(2H)-Benzofuranone dimethyl	162 (100) 104 (78) 77 (69) 51 (52) 131 (54) 76 (44) 135 (38) 165 (13)	3(2H)-Benzofuranone dimethyl	320
19 -	1264	ee	?	111 (100) 97 (98) 81 (92) 65 (75) 138 (67) 170 (33) 200 (32) 198 (18) 202 (2)		
20	1273	ee	p-Methoxypropylphenone	135 (100) 77 (27) 164 (22) 51 (16) 105 (10) 79 (9)		
21	1325	***	Phosphorodithioic acid, o,o-diethyl 8-ethyl	186 (100) 97 (76) 121 (61) 65 (56) 95 (57) 125 (25) 214 (24)		
22	1373	ee	$\text{C}_{10}\text{H}_{16}\text{O}$	202 (100) 187 (50) 145 (67) 159 (60) 91 (40) 203 (16)	Benzene, 1-(3,5-dimethyl-1-cyclopenten-1-yl)-2-methyl	323
23	1395	ee	?	86 (100) 81 (98) 111 (82) 55 (77) 135 (74) 165 (47) 191 (52) 224 (37)		
24	1452	ee	Mixture +	176 (100) 131 (98) 77 (91) 51 (82) 146 (84) 195 (72) 115 (65) 91 (66)		
25	1473	***	Homolog of #21	97 (100) 121 (93) 65 (76) 93 (71) 125 (64) 155 (49) 129 (44) 240 (50)		
26	1505	***	C_{10} -alkylphenol	107 (100) 135 (96)		
27	1529	***	?	55 (100) 123 (90) 106 (35) 63 (39) 124 (8) 192 (1)		
28	1582	***	Allyl-tetrahydrocaphthalene-1,1-diolide	146 (100) 176 (99) 121 (92) 195 (88) 77 (66) 51 (50) 91 (44) 218 (5)		
9	1605	ee	1,2-Benzisothiazole, 3-ethoxy	196 (100) 76 (56) 77 (52) 108 (37) 120 (28) 147 (23) 149 (17) 211 (14)	1,2-Benzisothiazole, 3-ethoxy, 1,1-diolide	642
20	1613	ee	" Isomer of #29	97 (100) 65 (74) 93 (53) 174 (42) 202 (46) 238 (74) 322 (16)		

TABLE A-119. (Continued)

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Elemental Analysis Compound	E.I. $\times 10^3$
31	1715	+++	Di-2-propenyl phthalate	149(100)41(52)104(46)76(44)132(37)189(49)190(6)	1,2-bis(2-propenyl)benzoic acid, di-2-	491
32	1768	+++	Subst.-benzofuranone	189(100)190(13)76(18)115(16)41(18)149(13)		
33	2121	++	?	199(100)103(60)76(39)135(38)61(24)162(23)		
34	2240	++	Sulfur-containing?	97(100)65(62)93(62)121(62)125(48)180(49)332(21)263(17)299(8)		
35	2379	+++	?	176(100)177(31)37(23)149(22)119(14)91(10)193(6)		
36	2611	++	Phthalate	149(100)		

TABLE A-120. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 45E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Elemental Analysis Compound	E.I. $\times 10^3$
1	876	++	Trimethylpiperidine	112(100)86(98)55(37)127(26)	Piperidine, 1,2,6-trimethyl-	434
2	882	++	Mixture ?	41(100)85(71)45(52)57(18)	2-Hexanone, 3,4-epoxy-	501
3	911	++	C ₈ -Alkylpiperidine MW 141	71(100)126(94)41(59)100(23)141(11)		
4	976	++	Methylpiperidine + ?	93(100)65(38)65(18)92(12)140(8)155(1)		
5	1056	+	Nethylaniline	106(100)107(76)122(11)77(20)91(5)		
6	1178	++	Nethoxyaniline MW 123	80(100)108(79)123(56)53(22)65(13)		
7	1344	++	Pentamethylbenzene MW 163	146(100)163(98)121(52)131(26)103(24)93(22)77(20)		

TABLE A-121. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 46VI

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44 (100)
2	0.16	>100	Dichloromethane	49 (100) 84 (100) Sat'd.
3	0.22	1-10	Chloroform	83 (100) 85 (65)
4	0.25	1-10	Dichloroethane	62 (100) 64 (33) 98 (15)
5	0.26	1-10	1,1,1-Trichloroethane	97 (100) 61 (70) 99 (67) 117 (15)
6	0.34	10-100	Dichloropropane	63 (100) 62 (70) 41 (50) 39 (35) 65 (30) 76 (23)
7	0.36	<1	Trichloroethylene	95 (100) 130 (80) 132 (79) 97 (63) 60 (45)
8	0.34	1-10	Toluene	91 (100) 92 (60)
9	0.68	<1	Tetrachloroethane	131 (100) 166 (95) 129 (80) 164 (73) 94 (61) 47 (48)
10	1.00	-(8)	IS	75 (100) 77 (33)

TABLE A-122. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 46VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.13	--	Air	44 (100)
2	.18	1-10	Dichloromethane	84 (100) 86 (70) 49 (50)
3	.29	1-10	1,1,1-Trichloroethane	97 (100) 99 (70) 61 (25) 117 (18)

TABLE A-123. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 47VI

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	---	air	44(100)
2	0.17	1-100	acetone	43(100)
3	0.18	10-100	Dichloromethane	49(100)
4	0.23	<1	Dichloroethylene *	61(100)96(72)98(50)63(30)
5	0.24	1-10	Isopropyl ether	45(100)43(50)41(15)87(12)
6	0.30	<1	benzene *	78(100)
			*Probably in blank	

TABLE A-124. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 47VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.14	---	Air	44(100)
2	.19	1-10	Diethylether	45(100)59(96)74(50)
3	.20	10-100	Dichloromethane	49(100)84(50)
4	.25	1-10	1,1-Dichloroethylene	61(100)96(45)
5	.27	1-10	Isopropyl ether	45(100)45(43)87(20)
6	.29	.1-1	Tetrahydrofuran	42(100)72(30)71(28)
7	.34	.1-1	Benzene	78(100)
8	.65	.1-1	Dichloropropane	76(100)41(47)78(40)
9	1.00	(8)-	I.S.	75(100)77(30)110(28)

TABLE A-125. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 48VI

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	---	Air	44 (100)
2	0.21	10-100	Dichloromethane	49 (100)
3	0.21	1-10	Cyclopentadiene	66 (100) 65 (65)
4	0.26	<1	Dichloroethylene	61 (100) 96 (52) 63, 98 (33)
5	0.27	<1	Chloroform	83 (100) 47 (80) 85 (60)
6	0.31	~1	1,1,1-trichloroethane	97 (100) 99 (63) 61 (50) 63 (18) 117, 119 (6) 121 (4)
7	0.41	~1	trichloroethylene	130 (100) 132 (97) 94 (94) 96 (62)
8	0.52	<1	acetylacetyl Ketone	43 (100) 58 (30) 85 (15) 100 (10)
9	0.58	<1	toluene	91 (100)
10	0.71	<1	1,1,2,2-tetrachloroethane	166 (100) 129 (90)
11	1.00	---	I S	75 (100)

TABLE A-126. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 48VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	---	Air	44 (100)
2	0.18	10-100	Dichloromethane	84 (100)
3	0.31	1-10	1,1,1-trichloroethane	97 (100) 99 (70) 61 (25) 119 (10) 117 (8) 121 (4)
4	1.00	---	I S	75 (100)

TABLE A-127. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 49VI

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	---	Air	44(100)
2	0.16	>100	Acetone	43(100)58(40)
3	0.17	10-100	C_4H_{10} , eg. 2-methyl-2-butene	55(100)70(28)41,42(20)
4	0.17	10-100	Diethyl ether (T) Sat'd	45,59,74(100)
5	0.17	10-100	Dichloromethane	49(100)
6	0.18	10-100	Carbon disulfide	76(100)
7	0.22	10-100	Dichloroethylene	61(100)96(60)98(40)63(35)
8	0.24	10-100	Chloroform	83(100)
9	0.28	<1	1,1,1-Trichloroethane	97(100)99(67)61(55)117,119(12)
10	0.28	1-10	2-Methyl-2-butanol	59(100)73(57)43(46)55(45)
11	0.30	---	Benzene	78(100)
12	0.31	10-100	Carbon tetrachloride	119(100)117(80)47(50)82(48)
13	0.34	1-10	Cyclohexane	67(100)54(70)82(40)41(25)
14	0.38	10-100	Trichloroethylene	95(100)130(82)132(79)60(62)
15	0.59	10-100	Toluene	91(100)92(60)
16	0.75	1-10	1,1,2,2-Tetrachloroethene	166(100)129,131(90)164(82)166(50)89(42)
17	0.84	1-10	Chlorobenzene	112(100)77(58)114(33)
18	0.90	1-10	C_2 Alkyl benzene	91(100)106(30)
19	0.93	10-100	C_2 Alkyl benzene	91(100)106(50)
20	0.97	1-10	Cyclooctatetraene	104(100)78(62)103(60)
21	0.98	1-10	C_2 Alkyl benzene	91(100)106(40)
22	1.00	----	I.S.	75(100)
23	1.05	1-10	Bromobenzene	156(100)158(98)77(75)
24	1.17	1-10	Butyl Ketone	85(100)57(88)41(35)142(20)127(10)

TABLE A-128. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 49VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.10	---	air	44(100)
2	0.13	>>>100	Diethyl ether	59(100)45(78)74(70)
3	0.15	10-100	Dichloromethane	49(100)
4	0.20	10-100	Chloroform	83(100)
5	0.22	>100	Tetrahydrofuran	42(100)41(55)71(50)72(50)
6	1.00	---	I S	75(100)
7	1.15	1-10	$\text{C}_{10}\text{H}_{16}$	93(100)91(58)92(45)77(30)79(25)105(20)121(15)

TABLE A-129. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 49I

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Name	R.I. $\times 10^3$
1	862	oo	Oxibicyclo[4.1.0]heptane	83(100)41(62)55(40)56(40)69(30)97(13)	7-Oxibicyclo[4.1.0]heptane	584
2	868	oo	Ethylbenzene	91(100)106(41)77(13)51(12)65(9)	Benzene, ethyl	779
3	872	oo	C_9 -Alkylbenzene + Alkyl alcohol	56(100)55(56)43(56)69(29)91(8)108(3)105(1)	1-Pentanol	635
4	1061	oo	Ethane, 1,1'-oxybis[2-ethoxy]	45(100)59(44)72(63)73(60)105(4)	Ethane, 1,1'-oxybis[2-ethoxy]	577
5	1130	oo	Dibromocyclohexane + ?	81(100)79(85)53(60)61(43)77(25)97(23)112(1)		
6	1165	oo	Bromocyclohexanol	81(100)79(20)53(46)61(13)117(10)127(6)119(3)	Cyclohexanol, 2-bromo	618
7	1209	oo	Dibromocyclohexane	83(100)55(44)111(33)41(28)67(10)196(8)	1,1'-Bicyclohexyl-2-ethyl-trans	306
8	1329	oo	1,1'-Bicyclohexyl-ethyl	95(100)55(80)113(62)41(58)67(46)112(29)83(26)114(5)178(1)		
9	1367	ooo	Subst. -cyclohexane	95(100)55(56)67(35)41(34)96(35)97(30)178(16)		
10	1677	o	? Isomer of #9	108(100)109(82)179(40)137(36)90(25)81(20)43(35)	Acetamide, N-(5-ethoxyphenyl)	816
11	1705	oo	N-(2-ethylphenyl)phthalate	169(100)167(29)57(36)70(22)71(22)		
12	2311	oo				

TABLE A-130. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 49I

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Monomer Methyl Compound	R.I. $\times 10^3$
1	1437	++	Benzenesulfonic acid, 4-methyl hydrosulfide	91 (100) 155 (59) 65 (48) 186 (59) 187 (4)		
2	1509	+	C $\geq$ 12 Fatty acid	74 (100) 87 (64)		
3	1615	++	Isomer of #1	91 (100) 85 (39) 121 (32) 155 (25) 185 (27) 186 (2)		
4	1709	+	C $\geq$ 16 Fatty acid	74 (100) 87 (75)		
5	1757	+	Methyl benzenesulfonamide	91 (100) 171 (52) 155 (50) 107 (48) 65 (88)	Benzenesulfonamide, 4-methyl	578
6	1886	+	C $\geq$ 15 Fatty acid		10-Undecenoic acid, methyl ester	616

TABLE A-131. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 49E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Monomer Methyl Compound	R.I. $\times 10^3$
1	863	++	Chlorobenzene	112 (100) 77 (79) 114 (31) 51 (31) 50 (30) 78 (5)	Benzene, chloro	582
2	932	+	Methylcyclohexanone	83 (100) 42 (66) 41 (66) 56 (44) 55 (43) 69 (30) 97 (12)	Cyclohexanone, 4-methyl	359
3	960	+	Chlorocyclohexane	57 (100) 87 (42) 55 (36) 41 (35) 54 (33) 118 (1) 120 (0.3)	Cyclohexane, chloro	564
4	999	+	Decane	57 (100) 43 (91) 71 (36) 25 (22) 99 (5) 142 (3)	Decane	889
5	1009	++	Chlorocyclohexanol	57 (100) 80 (26) 81 (19) 41 (18) 68 (12) 98 (9) 134 (4) 136 (1)	Cyclohexanol, 4-chloro	567
6	1015	++	Sibet., ketone	43 (100) 81 (50) 71 (43) 108 (33) 111 (30) 139 (18) 154 (18)	2-Quabicyclo[2,2,2]octan-1,3,3-trimethyl	707
7	1061	++	?	45 (100) 59 (43) 72 (60) 73 (30) 123 (10)		
8	1079	++	Cy-allylcyclopentane	81 (100) 87 (68) 88 (55) 99 (50) 110 (47) 93 (40) 124 (4) 152 (1)	Cyclopentane, 2-ethylidene-1,1-dimethyl	598
9	1099	+	Undecene	57 (100) 43 (93) 71 (46) 85 (22) 156 (2)	Dodecane	772
10	1130	++	Allyl-cyclohexene	81 (100) 79 (80) 53 (60) 77 (58) 105 (39) 51 (34) 148 (2)	Cyclohexene, 3-[2-propenyl]	608
11	1181	+++	Iodheptene	81 (100) 99 (50) 37 (40) 35 (36) 79 (30) 127 (8) 128 (4) 226 (2)		
12	1229	+++	Mixture of Isodichlorocyclohexane	53 (100) 67 (99) 81 (97) 117 (28) 127 (15) 244 (8) 246 (3)		
13	1348	+	1,1'-biphenyl	154 (100) 153 (40) 152 (27) 115 (21) 76 (17) 51 (16) 63 (14)		
14	1364	++	?	77 (100) 107 (67) 51 (36) 137 (24) 152 (20)		
15	1433	+	Bromonaphthalene	127 (100) 126 (20) 43 (22) 206 (74) 207 (71)	1,2-Dibromonaphthalene	575
16	1521	+	1,1'-Bicyclohexyl-2-ethyl	83 (100) 55 (50) 111 (96) 41 (20) 194 (5)	1,1'-Bicyclohexyl, 2-ethyl-, trans	308
17	1533	+	Mixture of #8	83 (100) 55 (86) 112 (55) 41 (50) 109 (38) 165 (32) 203 (4)		
18	1615	++	?	83 (100) 55 (86) 165 (58) 95 (59) 41 (49) 109 (42)		
19	2093	++	?	93 (100) 188 (56) 271 (2)		

TABLE A-132. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 49E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Compound	E.I. No.
1	1416	*	Indacolinidine, C ₂ Alkylphenyl	85(100)37(67)56(6)191(36)117(17)	Herpholine, 3,4-dimethyl-2-phenyl- (2R, Trans-)	361
2	1432	*	Indacolinidine, C ₃ Alkylphenyl	99(100)70(64)162(58)91(42)71(40)117(12)180(14)		
3	1480	ee	?	100(100)77(22)64(15)72(14)182(6)167(3)		
4	1545	ee	Isomer of #3	100(100)72(66)77(39)44(50)56(21)180(10)		
5	1913	ee	?	58(100)71(58)167(19)180(14)182(8)183(4)184(0.2)		

TABLE A-133. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 50VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.14	---	Air	44(100)
2	0.18	1-10	Dichloromethane	49(100)
3	0.24	<1	Chloroform	83(100)
4	0.36	<1	1,2-dichloropropane	63(100)62(70)41(55)71(50)65(30) Sm 97,99,112,114
5	0.64	1-10	1,2,2-trichloropropane	97(100)99,111(70)113(45) Sm 131,133,135
6	1.00	---	I S	75(100)
7	1.20	<1	C ₃ alkyl benzene	105(100)120(45)
8	1.21	<1	dichlorobenzene	146(100)148(70)111(33)75(25)
9	1.24	<1	C ₃ alkyl benzene	105(100)120(50)
10	1.35	<1	C ₄ alkyl benzene	119(100)134(30)
11	1.41	<1	C ₄ alkyl benzene	119(100)134(30)
12	1.41	<1	C ₄ alkyl benzene	119(100)134(40)
13	1.44	<1	C ₁₀ H ₁₂ eg C ₂ styrene	117(100)132(40)115(38)133(28)
14	1.45	<1	C ₄ alkyl benzene	119(100)134(40)
15	1.48	1-10	trichlorobenzene	180(100)182(95)184(40)145(25)147(15)

TABLE A-134. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 50E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Mass Spectrometric Search Compound	RI, $\times 10^3$
1	855	++	1,3-Dioxolane-2-(chloromethyl)	73 (100) 55 (46) 121 (16) 97 (6) 123 (5)	1,3-Dioxolane-2-(chloromethyl)	343
2	1003	++	2-Propanol, 1-(2-methoxy-1-methylethoxy)	59 (100) 55 (40) 103 (28) 73 (28) 106 (4)	2-Propanol, 1-(2-methoxy-1-methylethoxy)	711
3	1007	++	" Isomer of #2	59 (100) 55 (62) 73 (28) 103 (26)	"	672
4	1215	+++	Benzeneethanamine, N-methyl, H-microno	91 (100) 120 (63) 92 (48) 150 (28) 65 (20) 51 (10) 151 (3)	Benzeneethanamine, N-methyl, H-microno	376
5	1360	++	Microniline	65 (100) 136 (83) 92 (58) 89 (30) 55 (25) 118 (26) 139 (6) 121 (6)	Benzeneethanamine, N-microno	373
6	1501	++	Chloroalkylacet. -phenol	108 (100) 91 (64) 107 (36) 65 (22) 200 (16) 202 (5)		
7	1658	++	2,4-Bis(1-methylbutyl)-phenol	205 (100) 71 (26) 43 (26) 206 (16) 234 (6)	Phenol, 2,4-bis(1-methyl butyl)-	433
8	1676	++	C ₂ 16 Alkane	57 (100) 43 (70) 41 (42) 76 (59) 85 (47) 99 (14) 146 (4)	Pentacosane	646
9	1700	+++	"	44 (100) 68 (83) 201 (78) 186 (57) 173 (46) 96 (40) 203 (26) 214 (6)		
10	2337	++	"	91 (100) 117 (24) 65 (12) 155 (5) 147 (6) 207 (6) 208 (5)		
11	2511	++	Bis(2-ethylhexyl)phthalate	149 (100) 57 (44) 71 (28) 167 (28) 113 (10)	1,2-Benzenedicarboxylic acid, diisopropyl ester	368

TABLE A-135. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 50E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic line in Mass Spectrum	Most Reasonable Chemical Match Compound	K.I. $\times 10^3$
1	1268	*	Hydroxybenzoic acid	77(100)107(82)161(86)246(34)279(38)162(8)	Benzoic acid, <i>o</i> -hydroxy-methyl ester	515
2	1299	*	Trichlorophenol	195(100)197(96)198(30)167(76)169(72)210(50)212(46)214(15)	Benzene, 1,3,5-Trichloro-2-methoxy	764
3	1341	**	Benzenedicarboxylic acid monomethyl ester	41(100)91(45)180(41)107(30)121(29)77(16)65(13)181(2)		
4	1361	*	Triamethylbenzoic acid	147(100)146(64)178(37)119(36)91(34)165(13)	Benzoic acid, 2,4,5-Triamethyl-methyl ester	617
5	1364	**	Triamethylbenzoic acid	147(100)146(64)178(37)119(36)91(34)165(13)	Benzoic acid, 2,4,5-Triamethyl-methyl ester	560
6	1354	*	Hydroxy-triamethylbenzoic acid	105(100)133(79)134(56)77(50)144(60)136(40)193(4)		
7	1567	**	Chloro- ?	113(100)141(93)151(91)77(70)217(92)219(19)		
8	1628	**	Dichloro- ?	126(100)154(64)95(56)188(64)190(41)233(36)255(23)257(4)		
9	1705	**	Bromo- ?	246(100)248(100)75(81)62(72)276(42)278(42)		
10	1073	**	?	205(100)57(59)91(43)175(64)177(54)217(29)261(6)271(3)		
11	1906	***	?	41(100)147(64)161(16)277(35)292(16)219(15)293(2)		
12	2333	**	Chloro- ?	101(100)77(66)79(29)262(13)264(4)326(8)328(4)		
13	2399	**	Chloro- ?	106(100)77(78)90(48)126(24)296(16)197(14)232(12)296(6)		
14	2475	**	Chloro- ?	65(100)92(96)90(87)126(88)282(65)284(23)217(19)		

TABLE A-136. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 50E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic line in Mass Spectrum	Most Reasonable Chemical Match Compound	K.I. $\times 10^3$
1	977	***	Methylpyridine	93(100)146(100)56(40)92(40)94(23)163(18)157(16)	Pyridine, 3-Methyl	446
2	1067	**	Methylaniline	106(100)107(89)77(22)70(18)51(10)	Nenzenamine, 4-Methyl	626
3	1147	*	C ₆ -alkyl-pyridine	120(100)77(30)130(22)51(12)	1,2-Ethanediamine, N,N'-DiMethyl-N,N'-diphenyl-	523
4	1163	***	2-Methoxyaniline	80(100)108(80)123(33)33(18)	Nenzenamine, 2-Methoxy	706
5	1182	*	3-Methyl-5-Ethoxypyrazole	98(100)97(40)126(32)67(22)		
6	1195	**	Benzenesulfonamide, N-(aminocarbonyl)	118(100)91(36)134(32)116(26)165(15)178(16)179(2)	Benzenesulfonamide, N-(aminocarbonyl)-	228

TABLE A-137. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 51VI

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	--	Air	44(100)
2	0.17	1-10	Diethylether	59(100)45(98)74(58)
3	0.18	10-20	Dichloromethane	49(100)84(40)
4	0.24	~ 1	Chloroform	83(100)85(67)
5	0.25	1-10	1,1-di-propoxyethane (T)	45(100)43(45)87(22)59(15)95(6)
6	0.27	<1	Tetrahydrofuran	42(100)71,72(33)
7	0.28	1-10	Dichloroethane	62(100)49(38)64(33)98(12)
8	0.29	1-10	1,1,1-Trichloroethane	97(100)99(67)61(55)63(18)117,119(14)
9	0.38	80-100	Dichloropropane	63(100)62(70)41(50)65(30)76(28) Sm 112,114
10	0.40	~ 1	Trichloroethylene	95(100)130(78)132(76)97(63)134(33)
11	0.75	1-10	1,1,2,2-Tetrachloroethene	166(100)129(89)131(88)164(82)
12	1.00	-(8)	IS	75(100)77(33)

TABLE A-138. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 51VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44(100)
2	0.16	1-10	Chloropropene + Diethyl ether	74(100)59(85)41(78)39(65)45(30)76(27)78(10)
3	0.16	10-100	Dichloroethane	84(100)49(99)86(95)
4	0.19	<1	Methylpentane	43(100)42(55)41(33)71(22)86(2)
5	0.20	<1	C ₆ H ₁₄	57(100)41(82)56(78)43(53)72(9)86(4)
6	0.22	1-10	Chloroform	83(100)85(67)47(55)
7	0.24	<1	Tetrahydrofuran	42(100)41(80)39(45)55(38)72(35)71(34)
8	0.25	1-10	Dichloroethane	62(100)49(50)84(33)98(8)100(6)
9	0.26	<1	1,1,1-Trichloroethane	97(100)99(70)61(51)119(18)117(16)
10	0.34	10-100	Dichloropropene	63(100)62(70)41(50)39(35)65(30)76(26)
11	0.36	<1	Trichloroethylene	95(100)130(80)132(80)97(70)
12	0.45	<1	Tetramethylcyclopropane (T)	55(100)83(78)41(62)39,56(42)69(32)98(32)
13	0.49	<1	C ₆ H ₁₆ , e.g., Dimethylcyclohexane	55(100)97(67)69(45)112(20)
14	0.67	1-10	Tetrachloroethene	166(100)131(95)129(94)164(80)
15	1.00	-(8)	IS	75(100)77(33)

TABLE A-139. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 51E

GC Peak No.	Retention Index	Amount, µg ¹	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Benzene Match Compound	K.I. # 103
1	849	++	Chlorobenzene	112(100)77(76)114(32)51(29)50(28)74(12)	Benzene, chloro	598
2	999	+	Chlorocyclohexanol	57(100)80(26)81(18)98(9)105(3)134(2)116(1)	Cyclohexanol, 4-chloro	564
3	1051	+++	Nitrobenzene	77(100)51(70)123(26)50(20)65(16)91(14)	Benzene, nitro-	711
4	1073	+	Bromocyclohexanol	81(100)57(66)99(27)134(3)132(2)	Cyclohexanol, 2-bromo	472
5	1100	+	Bromochlorocyclohexane	81(100)78(18)53(13)41(12)117(6)118(2)	Cyclohexane, 1-bromo-2-chloro	451
6	1131	++	Nitrocyclohexane	81(100)79(66)53(69)41(51)97(21)127(4)		
7	1183	+	Baio-cyclohexane	81(100)89(29)41(28)57(26)55(25)79(23)127(5)128(3)		
8	1197	+	Baio-cyclohexane	81(100)41(33)35(29)57(24)79(23)98(7)		
9	1350	++	1,1'-Biphenyl	154(100)153(41)132(29)155(12)76(20)51(16)115(7)	1,1'-Biphenyl	581

TABLE A-141. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 52E

GC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic ions in Mass Spectrum	Most Reasonable Chemical Match Compound	E.I. X 10 ³
1	896	ee	Methoxybenzene	108 (100) 78 (79) 65 (74) 93 (18) 51 (16) 109 (6)	Benzene, Methoxy-	541
2	946	e	Chlorophenol	128 (100) 64 (35) 130 (32) 92 (16) 100 (8)	Phenol, 2-Chloro-	455
3	1002	eeee	Phenol	94 (100) 66 (85) 65 (56) 40 (64) 95 (12)	Phenol	470
4	1044	ee	Bromophenol + #6	108 (100) 107 (87) 77 (64) 79 (43) 90 (24) 172 (20) 174 (19)		
5	1047	ee	Benzoic Acid + #4	105 (100) 77 (60) 136 (36) 51 (20)	Benzoic Acid, Methyl Ester	413
6	1048	ee	Methylphenol	107 (100) 108 (82) 77 (36) 79 (24) 109 (6)	Phenol, 2-Methyl-	666
7	1091	ee	Chlorophenol (methylated)	142 (100) 99 (84) 107 (76) 127 (55) 108 (32) 77 (42) 144 (32) 63 (27)	Benzene, 1-Chloro-4-Methoxy	350
8	1135	ee	Dimethylphenol	107 (100) 122 (81) 121 (49) 91 (40) 77 (34) 150 (4)	Phenol, 2,4-Dimethyl	593
9	1169	ee	Bromomethoxybenzene	186 (100) 187 (97) 143 (59) 145 (58) 63 (42) 92 (30) 171 (41) 172 (40)	Benzene, 1-Bromo-2-Methoxy	412
10	1178	ee	Methylbenzoic Acid	119 (100) 91 (58) 150 (37) 107 (28) 85 (20) 186 (2) 188 (2)	Benzoic Acid, 3-Methyl-Methyl Ester	321
11	1285	ee	Trichlorophenol (methylated)	185 (100) 197 (97) 167 (61) 149 (59) 210 (54) 212 (51) 214 (17) 97 (20)	Benzene, 1,2,4-Trichloro-5-Methoxy	583
12	1626	ee	Benzene sulfonamide H, A-Dimethyl	91 (100) 85 (28) 155 (24) 121 (21) 185 (22)	Benzene Sulfonamide, H, A-Dimethyl	591
13	1818	ee	Phenol, 2,4-(4-Hydroxyphenyl)dimethyl	108 (100) 52 (18) 77 (12) 91 (11) 214 (36) 181 (24) 183 (7)		
14	1944	ee	Phenol, 2-(4-(Hydroxyphenyl)methyl)-	107 (100) 94 (36) 77 (20) 152 (18) 200 (56) 181 (15) 165 (4)	Phenol, 2-(4-(Hydroxyphenyl) Methyl]	596
15	1978	ee	C ≥ 18 Fatty Acid	74 (100) 87 (84) 143 (26) 199 (9) 253 (4) 298 (3)	Septadecanoic Acid, 16-Methyl, Methyl	583
					Ester	
16	2035	ee	Phenol 2-(4-(Hydroxyphenyl)methyl]	107 (100) 77 (28) 152 (18) 153 (16) 200 (65) 199 (41) 201 (11)	Phenol, 2[(4-(Hydroxyphenyl) Methyl]	522
17	2302	ee	1-Phenanthrenecarboxylic Acid Octahydro.	239 (100) 240 (19) 197 (15) 141 (20) 129 (17) 150 (16) 299 (11) 314 (5)	1-Phenanthrenecarboxylic Acid Octahydro,	696
			1,4-Dimethyl-7-(1-Methylethyl) Methyl		1,4-Dimethyl-7-(1-Methylethyl) Methyl	
			Ester		Ester	

TABLE A-142. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 52E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Element Match Compound	R.I. ± 10°
1	866	***	Cyclohexylamine	56 (100) 43 (26) 99 (20) 70 (11)	Cyclohexan amine	595
2	890	***	Hydroxyethylamine	56 (100) 98 (66) 81 (42) 62 (32) 53 (32) 49 (31) 97 (35) 99 (20)		
3	971	***	Ethanol, 2-(Diethylamine)	86 (100) 58 (60) 42 (17) 102 (13) 117 (7)	Ethanol, 2-Diethylamine	541
4	1032	**	Methylpyridine	93 (100) 66 (37) 65 (16) 92 (12) 94 (6)	Pyridine, 3-Methyl	512
5	1381	**	5-Hexen-3-yn-2-one, 6-(1-Piperidinyl)	96 (100) 148 (77) 134 (65) 177 (50) 122 (38) 52 (32) 81 (27)	5-Hexen-3-yn-2-one, 6-(1-piperidinyl)	402
6	2017	*	1,2-Dicyclohexylurea	56 (100) 55 (43) 99 (42) 143 (41) 98 (26) 224 (14)		

TABLE A-143. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 53VE

GC Peak No.	Relative Retention Time	Amount, μ g/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	--	Air	44(100)
2	0.13	<1	Butene	41(100)56(70)39(41)
3	0.15	10-100	Acetone	43(100)58(25)
4	0.16	1-10	Dichloroethylene	61(100)96(90)98(55)63(33)
5	0.17	10-100	Dichloromethane	49(100)84(45)
6	0.18	10-100	Carbon disulfide	76(100)78(6)
7	0.21	1-10	Dichloroethylene	61(100)96(40)83(30)98(25)
8	0.22	10-100	Chloroform	83(100)85(60)47(55)
9	0.26	1-10	Trichloroethylene	97(100)61(90)99(60)117(6)
10	0.26	1-10	Methylbutyl aldehyde (T)	44(100)41(76)43(62)58(52)71(20)86(3)
11	0.28	1-10	Benzene	78(100)
12	0.32	1-10	C ₇ H ₁₆	43(100)41(50)56(49)57(40)85(18)71(15)100(2)
13	0.35	1-10	Bromodichloromethane	83(100)85(65) Small 127, 129, 131
14	0.35	1-10	Trichloroethylene	95(100)97(70)60(65)130(40)132(40)
15	0.53	10-100	Toluene	91(100)92(55)
16	0.56	10-100	Tetramethyltetrahydrofuran (T)	43(100)55(35)70(30)113(21)59(15)95(10)
17	0.68	1-10	Tetrachloroethylene	166(100)131(94)129(80)164(78)94(65)96, 168(40)
18	0.88	<1	C ₂ Alkylbenzene	91(100)106(30)
19	0.90	1-10	C ₂ Alkylbenzene	91(100)106(40)
20	0.98	1-10	C ₂ Alkylbenzene	91(100)106(40)
21	1.00	-(8)	IS	75(100)
22	1.07	<1	C ₉ H ₂₀	43(100)57(70)85(15)71(14) Sm 128

TABLE A-144. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 53E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Yenative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Structure Match	E.I. $\times 10^3$
1	886	***	Phenol	94 (100) 66 (44) 65 (27) 55 (6) 95 (6)	Phenol	539
2	944	**	Chlorophenol + Methylphenol	108 (100) 107 (96) 77 (48) 79 (43) 51 (18) 90 (22) 142 (6) 144 (2)	Phenol, 2-Methyl-	522
3	958	**	Benzoic Acid + Bromophenol	105 (100) 77 (64) 136 (36) 51 (26) 172 (16) 174 (14)	Benzoic Acid, Methyl Ester	247
4	988	**	Methylphenol	107 (100) 108 (83) 77 (56) 79 (25) 51 (12) 55 (10)	Phenol, 2-Methyl-	445
5	997	**	Chloromethylphenol + #4	107 (100) 108 (56) 77 (61) 142 (27) 144 (8)	Phenol, 4-Chloro-2-Methyl-	350
6	1049	**	C $\geq$ 7 Fatty Acid	74 (100) 87 (46) 55 (24) 59 (18) 115 (8)	Hexanoic Acid, 5-Methyl-, Methyl Ester	359
7	1099	**	Benzenedicarboxylic Acid	91 (100) 130 (27) 65 (18) 99 (8) 59 (6)	Benzenedicarboxylic Acid, Methyl Ester	652
8	1110	**	Methylbromophenol + 7	107 (100) 77 (60) 120 (56) 92 (43) 132 (26) 146 (60) 188 (59)		
9	1215	**	Benzenetricarboxylic Acid	104 (100) 91 (56) 105 (37) 164 (28) 77 (22) 128 (16) 95 (14) 51 (10) 131 (8)	Benzoic Propionic Acid, Methyl Ester	507
10	1288	**	Trichlorophenol + Fatty Acid	74 (100) 87 (62) 143 (20) 55 (20) 59 (14)	Dodecanoic Acid, Methyl Ester	260
11	1354	**	Methylbromophenol	107 (100) 186 (84) 188 (84) 77 (76) 51 (24) 121 (10) 151 (8)	Dodecanoic Acid, Methyl Ester	653
12	1504	**	Dodecanoic Acid	74 (100) 87 (71) 55 (20) 43 (17) 143 (14) 214 (2)	Tetradecanoic Acid, Methyl Ester	607
13	1707	**	Tetradecanoic Acid	74 (100) 87 (76) 55 (22) 43 (20) 143 (20) 199 (10) 242 (1)	Tetradecanoic Acid, 12-Methyl-Methyl Ester	422
14	1808	**	Pentadecanoic Acid	74 (100) 87 (82) 43 (18) 55 (24) 143 (21) 210 (10) 256 (2)	10-Undecanoic Acid, Methyl Ester	408
15	1883	**	C $\geq$ 15 Fatty Acid	55 (100) 74 (70) 87 (51) 236 (3) 237 (2)	Hexadecanoic Acid, Methyl Ester	689
16	1913	***	Heptadecanoic Acid	74 (100) 87 (86) 43 (24) 55 (22) 143 (20) 270 (2) 319 (1)	Heptadecanoic Acid, 14-Methyl-, Methyl Ester	508
17	2010	**	C $\geq$ 17 Fatty Acid	74 (150) 87 (82) 43 (23) 43 (31) 55 (24) 241 (4) 284 (2)	Ester	
18	2070	**	Octadecadecanoic Acid	67 (100) 81 (90) 55 (59) 95 (60) 109 (30) 286 (2) 262 (2) 263 (1)	9,11-Dichloro-11-oxo-11-undecanoic Acid, Methyl Ester	528
19	2083	***	Octadecanoic Acid	55 (100) 69 (74) 74 (72) 87 (57) 97 (56) 264 (7) 265 (5) 296 (1)	9-Octadecanoic Acid, Methyl Ester	742
20	2114	***	C $\geq$ 18 Fatty Acid	74 (100) 67 (82) 43 (24) 199 (8) 255 (4) 298 (3) 267 (1) 269 (0.5)	Heptadecanoic Acid, 16-Methyl-, Methyl Ester	702
21	2330	**	C $\geq$ 18 Fatty Acid	169 (100) 87 (83) 55 (68) 74 (58) 129 (28) 143 (25) 172 (16) 201 (10)	Ester	
22	2415	*	C $\geq$ 18 Fatty Acid	74 (100) 87 (90) 143 (30) 283 (4) 326 (4)	Hexadecanoic Acid, Methyl Ester	508
23	2518	*	C $\geq$ 19 Fatty Acid	74 (100) 87 (86) 143 (28)	Triscontanoic Acid, Methyl Ester	507

TABLE A-145. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 53E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Yenative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Structure Match	E.I. $\times 10^3$
1	865	***	N,N-Dimethylacetamide	87 (100) 44 (86) 43 (55) 42 (42) 72 (40) 88 (6)	N,N-Dimethylacetamide	623
2	1205	**	Quinoline	129 (100) 102 (90) 128 (21) 130 (10) 74 (12) 76 (12) 90 (9)	Quinoline	739

TABLE A-146. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 54VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Reference Identification	Characteristic Ions in Mass Spectrum
1	0.12	---	Air	44(100)
2	0.15	10-100	Acetone	43(100) 58(33)
3	0.16	10-100	Dichloroethylene	61(100) 96(60) 163(33) 98(32)
4	0.16	>100	Need better spectrum	51(100) 35(82) 147(68) 48(32) 37(23) 55(10) 70(5)
5	0.19	<1	1,2-Dichloroethane	63(100) 42(78) 85(30) 55(20)
6	0.19	1-10	2-Methylpentane	43(100) 42(50) 41(32) 71(20) 39(12)
7	0.20	1-10	3-Methylpentane	57(100) 56(80) 41(65) 43(64) 72(9) 71(5) 86(3)
8	0.21	1-10	Dichloroethylene	61(100) 96(52) 163(33) 98(30)
9	0.22	<10	Chloroform	83(100) 85(67)
10	0.24	<1	Tetrahydrofuran + C_6H_{12}	41(100) 69(57) 42(50) 39, 84(23)
11	0.25	1-10	Methyl cyclopentane	56(100) 41(65) 69(30) 55(22) 84(4)
12	0.26	10-100	1,1,1-Trichloroethane	97(100) 99(66) 117(12) 119(10)
13	0.28	10-100	Benzene	78(100)
14	0.30	<1	Cyclohexane	56(100) 41(65) 84(48) 55(32) 69(25)
15	0.33	<1	Alkane	43(100) 41(55) 56(50) 57(40) 42(32) 71(15) 85(8)
16	0.34	<1	C_7H_{16} Alkane	43(100) 41, 57(46) 71(41) 56, 70(32) 85(5) 100(2)
17	0.36	10-100	Trichloroethylene	95(100) 97(67) 130(60) 132(58)
18	0.41	<1	C_7H_{16} Alkane	43(100) 41(60) 57(40) 71(35) 100(10)
19	0.46	1-10	C_7H_{16} Alkane	55(100) 83(80) 41(61) 42(38) 98(30)
20	0.55	10-100	Toluene	91(100) 92(60)
21	0.68	<1	C_8H_{16}	55(100) 41(55) 97(50) 56(32) 42(20) 68(21) 83(11) 112(10)
22	0.69	1-10	1,1,2,2-Tetrachloroethane	129(100) 166(95) 131(90) 164(70) 94(75)
23	0.70	<1	C_8H_{16}	55(100) 57(60) 41(45) 112(15)
24	0.73	1-10	C_8H_{18} Alkane	43(100) 57(30) 85(20) 71(15) Sm 114
25	0.80	<1	Chlorobenzene	112(100) 77(95) 51(40)
26	0.82	1-10	C_8H_{16}	55(100) 83(75) 41(62) 82(38) 112(10)
27	0.87	<1	Alkane	57(100) 43(48) 41(40) 97, 99(10)
28	0.88	10-100	C_2 Alkyl benzene	91(100) 106(30)
29	0.89	<1	C_8H_{18}	69(100) 55(90) 111(60) 41(55) 56(40) 126(12)
30	0.91	10-100	C_2 Alkyl benzene	91(100) 106(40)

TABLE A-146. (Continued)

GC Peak No.	Relative Retention Time	Amount, µg/l	Testative Identification	Characteristic Ions in Mass Spectrum
31	.93	<1	Hydrocarbon	43(100)84, 41(22)85(18)57(17)
32	.96	A1	C ₉ H ₁₈	43(100)57(25)85(15)111(8)126(5)
33	.97	<1	C ₂ Alkyl benzene Y ?	55(100)91(60)106(30)
34	.98	10-100	C ₂ Alkyl benzene	91(100)106(45)
35	1.00	~(8)	T5	75(100)
36	1.00	1-10	C ₉ H ₁₈ Alkene	55(100)97(40)94(38)89(18)126(3)
37	1.05	1-10	C ₉ H ₁₈ Alkene	55(100)97(62)94(40)69(30)126(10)
38	1.07	1-10	C ₉ H ₂₀ Alkene	43(100)57(68)85(12)71(11)128(1)
39	1.08	1-10	C ₃ Alkyl benzene	105(100)120(25)
40	1.12	1-10	? Alkyl benzene	55(100)83(85)82, 41(45)126(5)
41	1.16	10-100	C ₃ Alkyl benzene	91(100) 120(12)
42	1.16	1-10	Alkene	57(100)43(70)71(55)94(50)56(30)113(8)
43	1.18	10-100	C ₃ Alkyl benzene	105(100)120(32)
44	1.18	10-100	C ₃ Alkyl benzene	105(100)120(30)
45	1.20	10-100	C ₃ Alkyl benzene	105(100)120(50)
46	1.22	10-100	C ₃ Alkyl benzene	105(100)120(30)
47	1.24	1-10	C ₁₀ H ₂₀ , eg. C ₆ Alkylcyclohexane	55(100)97(50)96(30)81(15)140(3)
48	1.25	10-100	C ₃ Alkyl benzene	105(100)120(40)
49	1.27	~10	Dichloro benzene	146(100)148(65)111(50)113(18)150(16)
50	1.29	1-10	C ₄ Alkyl benzene	91(100)134(20)
51	1.29	1-10	C ₄ Alkyl benzene	105(100)134(20)
52	1.32	10-100	Dichlorobenzene + Alkene	43(100)57(80)94(42)71(32)146(25)148(7)
53	1.33	1-10	C ₄ Alkyl benzene	119(100)91(32)136(22)
54	1.33	A10	Methyl Styrene	117(100)118(53)135(32)91(22)119(16)
55	1.35	~10	C ₁₀ H ₁₆ e.g. Limonene	68(100)67(77)93(40)107(11)121(10)136(5)
56	1.37	~10	Hydrocarbon	43(100)57(70)71(70)83(50)
57	1.38	~10	C ₄ Alkyl benzene	105(100)119(90)136(40)
58	1.38	10-100	C ₄ Alkyl benzene	105(100)134(20)

TABLE A-147. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 54E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Identifiable Component		R.I. $\times 10^3$
					Compound		
1	858	oo	Xylene	91(100)106(42)			
2	863	oo	C ₈ -Alkylbenzene	105(100)118(6)127(13)			
3	869	oo	C ₉ -Alkylbenzene	105(100)118(28)127(18)			
4	874	oo	C ₉ -Alkylbenzene	105(100)140(99)141(90)120(44)77(20)91(17)121(4)			
5	889	oo	C = 10 alkene	11(100)50(96)37(58)71(28)85(18)142(2)			
6	901	oo	C ₉ -Alkylbenzene	105(100)120(56)77(15)91(13)51(0)65(6)			
7	937	oo	C ₉ -Alkylbenzene	119(100)134(34)91(23)			
8	973	oo	C ₉ -Alkylbenzene	119(100)134(22)			
9	981	oo	C = 11 alkene	42(100)43(96)41(94)37(94)71(97)85(54)156(5)137(0.3)	Decane, 4-methyl		411
10	1005	oo	C ₉ -Alkylbenzene	119(100)140(88)134(35)91(24)	Benzene, 1-methyl-4-(1-methyl ethyl)		375
11	1089	oo	C ₉ -Alkylbenzene	133(100)119(61)91(33)148(33)			
12	1103	ooo	Dodecane	57(100)42(98)43(92)41(86)58(88)71(92)85(90)170(6)			
13	1204	ooo	Tridecane	42(100)41(89)43(67)37(84)71(70)98(16)85(14)184(0.3)	Tridecane, 4, 8-dimethyl		440
14	1248	ooo	Methyl-naphthalene	142(100)141(97)41(82)115(60)143(13)160(2)	Naphthalene, 1-methyl		276
15	1283	oo	Methyl-naphthalene	142(100)141(99.5)41(82)115(69)143(14)			
16	1304	ooo	Tridecane	43(100)57(96)71(96)85(91)99(18)184(4)185(0.2)	Tridecane		378
17	1367	oo	C > 13 Alkene	43(100)57(63)141(63)71(71)85(20)115(18)156(24)193(3)			
18	1381	ooo	C > 13 Alkene	43(100)57(96)71(88)85(48)117(12)127(12)183(1)			
19	1393	oo	Dimethylnaphthalene	156(100)141(87)115(77)128(20)155(35)157(12)	Naphthalene, 1, 2-dimethyl		462
20	1403	ooo	Dimethylnaphthalene + Tetradecane	58(100)44(99.5)85(96)71(90)141(76)156(77)198(4)			
21	1448	ooo	C > 14 Alkene + ?	85(96)71(88)37(82)58(79)55(66)99(33)141(11)183(3)			
22	1505	ooo	Pentadecane	71(100)58(99)44(99)85(90)99(24)155(20)212(1)			
23	1524	oo	C > 15 Alkene	43(100)57(58)55(56)83(68)97(16)169(7)			
24	1550	oo	C > 15 Alkene + ?	43(100)57(50)71(68)85(30)			
25	1604	ooo	Hexadecane	71(100)58(99)44(96)85(84)99(43)113(24)169(11)227(1)	Hexadecane		306
26	1655	ooo	C > 16 Alkene	58(100)42(91)85(82)71(74)99(20)113(26)169(10)			
27	1705	ooo	Heptadecane	71(100)58(99)44(99)85(88)99(42)113(24)127(14)240(1)			
28	1715	ooo	C > 17 Alkene	71(100)58(98)44(81)85(80)99(35)113(42)127(16)			
29	1805	ooo	Octadecane	71(100)58(99)44(98)85(88)99(46)113(28)			
30	1817	oo	C > 18 Alkene	43(100)71(86)37(76)85(75)113(23)127(18)	Heptadecane, 2, 6, 10, 14-tetramethyl		500

TABLE A-147. (Continued)

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Benzene Match Compound	R.I. $\times 10^3$
31	1906	++	Nicotrazine	43(100) 56(98) 85(90) 71(64) 99(37) 113(22) 127(13)		
32	2003	++	Fluorene	43(100) 85(96) 71(96) 57(80) 99(31) 113(19) 127(12)	Fluorene, 10-methyl	510
33	2106	++	Benzoic acid	41(100) 57(94) 71(64) 85(42) 99(12) 113(6)		

TABLE A-148. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 54E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Benzene Match Compound	R.I. $\times 10^3$
1	922	+++	Methylpyridine	93(100) 66(33) 65(17) 92(12) 94(7)	Pyridine, 3-methyl-	507
2	1034	++	Methyl aniline	106(100) 107(80) 77(30) 78(25) 51(16) 65(13)	Benzenamine, N-methyl	607
3	1061	++	Dimethylaniline	120(100) 127(72) 77(30) 104(18) 105(16) 51(12) 122(6)	1,2-Ethanedifluorene, N,N'-dimethyl-N,N'-diphenyl	601
4	1100	+	Cy-4-ethylpyridine	106(100) 121(34) 77(24) 65(12) 51(11) 127(5) 134(2)	Benzenamine, N-ethyl-	530
5	1135	++	Dimethylaniline	121(100) 106(98) 120(96) 77(23) 95(18) 65(9) 51(10)	Pyridine, 3-ethyl-5-methyl	427
6	1167	++	Chlorotoluene	121(100) 129(32) 65(26) 92(19) 100(14)	Benzenamine, 4-chloro	625
7	1200	+	N,N-Diethylamine	134(100) 106(50) 77(36) 149(27) 51(10)		
8	1255	++	Acetamide, N-(4-bromophenyl)	171(100) 173(100) 65(51) 92(45) 142(20) 141(17)		
9	1316	+	Pyridine 3-(1-methyl-2-pyrrolyldiyl)	94(100) 133(48) 141(26) 162(21)	Pyridine, 3-(1-methyl-2-pyrrolyldiyl)	632

TABLE A-149. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 55VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1.	.13	--	Air	44(100)
2	.15	500-1000	Acetone	43(100)58(40)
3	.16	1-10	Unknown (weak)	45(100)43(63)46(37)41(12)53(5)55(6)
4	.17	500-1000	Dichloromethane	49(100)84(40)
5	.23	~20	Chloroform	83(100)85(67)
6	.24	~10	Diisopropyl ether	45(100)43(40)87(18)59(12)69(4)
7	.26	<1	Tetrahydrofuran	42(100)71(30)41,72(30)85(10) ?
8	.27	<1	1,1,1-Trichloroethane	97(100)61(80)99(67)
9	.30	~1	Benzene	78(100)
10	.35	1-10	Cyclohexene	67(100)54(78)39(46)41,82(38)
11	.37	1-10	Bromodichloromethane	83(100)85(60)47(28)129(8)
12	.46	1-10	C ₈ H ₁₈ , e.g. Trimethyl pentene	57(100)41(50)55(30)69,97,112(6)
13	.57	>>100	Toluene	91(100)92(60)
14	.61	<1	Dibromochloromethane	129(100)127(80)131(40)
15	.89	1-10	Ethyl benzene	91(100)106(30)
16	.92	1-10	m,p-xylene	91(100)106(42)
17	.98	1-10	o-Xylene	91(100)106(40)
18	1.00	~(8)	I.S.	75(100)77(33)
19	1.26	10-20	Dichlorobenzene	146(100)148(66)75,111(54)
20	1.31	10-20	Dichlorobenzene	146(100)148(62)75,111(63)

TABLE A-150. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 56VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.11	--	Air	44(100)
2	.14	~ 10	Trichlorofluoromethane	101(100)103(67)
3	.16	10-100	Dichloromethane	49(100)84(60)
4	.22	>100	Diallopropyl ether	43(100)45(100)41,87(44)59(28)
5	.29	10-100	Benzene	78(100)
6	.35	1-10	Bromodichloromethane	83(100)85(67)129(6)127(4)
7	.54	10-100	Toluene	91(100)92(60)
8	.79	10-100	Chlorobenzene	112(100)77(90)114(33)
9	.88	1-10	C ₂ Alkyl benzene	91(100)106(30)
10	.91	1-10	C ₂ Alkyl benzene	91(100)106(45)
11	.98	1-10	O-xylene	91(100)106(42)
12	1.00	-(8)	I.S.	75(100)77(33)
13	1.25	10-100	Dichlorobenzene	146(100)148(67)
14	1.29	~ 10	Dichlorobenzene	146(100)148(67)

TABLE A-151. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 56E

GC Peak No.	Retention Index	Amount, µg	Tentative Identification	Characteristic Ions in Mass Spectrum	Major Nonvolatile Residual Masses Compound	R.I. ± 10
1	66.1	*	Chlorobenzene	112(100)77(68)114(34)50(28)31(25)	Benzene, chloro	571
2	66.7	*	Xylene	91(100)39(42)106(29)37(14)		
3	87.3	**	Xylene	91(100)106(44)105(23)77(14)		
4	89.9	***	$\text{CH}_3\text{CH}_2\text{-O-(CH}_2\text{)}_8\text{-C}_2\text{H}_5$ p-lymer	76(100)74(50)41(35)105(20)135(2)	Benzene, 1,2-dimethyl	563
5	92.1	**	Homolog of #4	45(100)75(70)105(20)135(7)		
6	98.7	*	Dichlorobenzene	146(100)148(64)111(31)75(48)113(18)150(11)	Benzene, 1,4-dichloro	561
7	100.8	*	Dichlorobenzene	146(100)148(63)111(32)75(48)30(28)150(11)	Benzene, 1,2-dichloro	502
8	103.5	*	Dichlorobenzene	146(100)111(50)148(44)67(37)		
9	107.8	***	Homolog of #4	105(96)91(28)135(14)107(14)		
10	110.8	***	?	61(100)41(85)91(34)43(30)121(2)		
11	112.2	**	?	78(100)106(43)136(28)31(20)137(2)		
12	114.9	*	Trichlorobenzene	180(100)182(97)74(46)109(40)145(39)184(30)147(26)	Benzene, 1,2,4-trichloro	647
13	118.1	*	Trichlorobenzene	180(100)	Benzene, 1,2,4-trichloro	450
14	125.6	***	Homolog of #4	45(100)75(79)105(30)107(13)135(10)		
15	129.7	**	?	112(100)77(93)140(63)31(43)114(32)142(24)170(24)172(12)		
16	143.1	***	Homolog of #4	45(100)75(75)105(43)107(20)135(20)165(2)		
17	159.1	**	Homolog of #4	45(100)75(70)105(56)135(33)107(22)165(5)		
18	160.5	***	Homolog of #4	135(100)105(100)107(89)91(55)121(37)165(13)		
19	177.6	**	Homolog of #4	45(100)75(80)105(70)135(43)165(12)185(2)		
20	195.5	**	Homolog of #4	45(100)75(70)105(60)135(44)165(26)185(3)		

TABLE A-152. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 56E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Match Compound	E.I. $\times 10^3$
1	909	***	Mixture	61(100) 91(34) 60(26) 44(10) 89(16) 121(1)		
2	989	*	Chlorophenol	128(100) 130(32) 64(35) 63(29) 92(16)	Phenol, 2-Chloro-	493
3	1017	***	Phenol	94(100) 66(50) 65(30) 40(26) 95(6)	Phenol	473
4	1038	**	Polymer ?	45(100) 75(84) 105(28) 135(6) 107(6)		
5	1070	**	Chlorobenzoic Acid	105(100) 77(70) 134(33) 51(26) 172(6) 174(6)	Benzoic Acid, Methyl Ester	453
6	1101	**	Mixture	61(100) 91(22) 44(11) 107(10) 108(9) 121(1) 119(0.5)		
7	1143	*	Dichlorophenol + ?	120(100) 92(77) 132(49) 83(28) 161(32) 176(30) 178(18)		
8	1169	**	Homolog of #4	45(100) 75(64) 105(35) 135(11) 117(10) 136(1)		
9	1241	**	Homolog of #4	45(100) 75(68) 105(48) 135(22) 107(18) 165(1)		
10	1818	**	Phenol, 2,6-[4-(Hydroxyphenyl)dimethyl]	108(100) 214(41) 181(26) 152(20) 77(15) 215(6)		
11	1967	**	Phenol, 2-[4-(Hydroxyphenyl)methyl]-	107(100) 200(70) 94(37) 77(27) 132(23) 181(20) 201(10)	Phenol, 4,4'-Methylenebis-	490
12	2009	**	Heptadecanoic Acid + ?	55(100) 74(69) 87(54) 200(26) 264(6)		
13	2040	**	C $\geq$ 17 Fatty Acid	74(100) 87(83) 143(24) 199(10) 255(4) 298(2)	Heptadecanoic Acid, 16-Methyl Ester	548

TABLE A-153. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 56E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Match Compound	E.I. $\times 10^3$
1	882	***	Mixture ?	82(100) 55(68) 68(47) 83(42) 96(11) 110(4)	Hexamethylenetriamine, 2-Methyl	402
2	916	***	Mixture ? PM 121	61(100) 91(55) 61(28) 89(20) 121(4)		
3	991	**	Isomer of #2	61(100) 91(27) 44(13) 60(10) 121(2)		
4	1059	**	Hexamethylacetamide	42(100) 140(75) 85(22) 112(12) 141(6)		
5	1100	**	Hexamethylacetamide	42(100) 140(75) 85(22) 112(12)		
6	1291	**	Homolog #2	61(100) 91(34) 89(31) 119(6) 121(4) 149(1)		

TABLE A-154. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 57VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	---	Air	44(100)
2	.13	1-10	Unknown	50(100)44(5)45(3)
3	.16	~100	Trimethyl Silanol	75(100)45(98)
4	.22	~30	Chloroform	83(100)85(67)
5	.22	~10	Diisopropyl ether	45(100)43(42)87(15)39(12)
6	.29	>>100	Benzene	78(100)
7	.53	1-10	Toluene	91(100)92(55)
8	.80	~100	Chlorobenzene	112(100)77(85)114(35)
9	1.00	~(8)	I.S.	75(100)77(33)
10	1.14	~80	Chlorotoluene	91(100)126(28)128(10)
11	1.15	1-10	Chlorotoluene	91(100)126(21)128(7)
12	1.26	20-30	Dichlorobenzene	146(100)75(77)111(67)148(65)
13	1.27	100-200	Dichlorobenzene	146(100)148(67)111(55)75(52)
14	1.30	80-100	Dichlorobenzene	146(100)148(67)111(60)75(52)

TABLE A-155. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 57E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Monomer Match Compound	R.I. # 103
1	902	+++	Methylphenol	108(100)78(86)45(80)93(20)51(18)109(11)	Benzene, Methoxy-	536
2	1007	+++	Chlorophenol + Phenol	66(100)96(99)65(92)55(24)50(19)128(8)130(2)	Phenol	433
3	1074	++	Benzoic Acid	105(100)77(98)136(78)51(46)50(21)	Benzoic Acid, Methyl Ester	541
4	1093	++	Chloromethylphenol	142(100)99(86)127(56)144(32)101(29)129(19)	Benzene, 1-Chloro-4-Methoxy	636
5	1172	++	Bromomethylphenol	186(100)168(96)143(65)145(63)171(41)173(40)63(34)77(18)	Benzene, 1-Bromo-2-Methoxy	637
6	1212	++	Phenylethanol	94(100)138(30)77(30)66(20)56(11)130(2)	Ethanol, 2-Phenoxy-	635

TABLE A-156. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 58VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.13	<10	Propene (T)	41(100)39(80)42(70)40(28)
3	.16	100-200	Acetone	43(100)58(100) (Sat'd)
4	.17	100-200	Isopropyl alcohol	45(100)41(22)43(20)
5	.23	1-10	Chloroform	83(100)85(65)
6	.27	<1	1,1,1-Trichloroethane	97(100)6(75)99(65)117,119(12)
7	.53	1-10	Unknown	59(100)43(77)77(22)103(15)
8	.55	1-10 ea	Toluene + Unknown	39(100)63(75)91(40)41(33)65(27)92(23)
9	.56	<1	Chloropropene	76(100)41(35)78(30)
10	1.00	-(13)	I.S.	75(100)77(33)

TABLE A-157. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 58E

GC Peak No.	Retention Time, min	Amount, µg ^b	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Monomer Methyl Compound	RT s. 193
1	1116	++		78 (100) 106 (70) 136 (51) 51 (40)		
2	1284	++	Benzeneethanol, methoxy-acetate	120 (100) 91 (95) 92 (78) 77 (20) 180 (18) 149 (13) 95 (13)	Benzeneethanol, <i>dl</i> -methoxy-acetate	404
3	1452	++	Mixture of Alkylbenzene	91 (98) 147 (96) 119 (96) 55 (78) 57 (76) 162 (46) 132 (24)		
4	1640	++	Chloro-hydrocarbon	41 (100) 55 (32) 37 (32) 91 (25) 68 (19) 71 (18) 105 (8)		
5	1780	++	?	177 (100) 91 (35) 108 (33) 77 (26) 57 (21) 192 (11) 228 (11)		
6	1978	++	?	134 (100) 57 (72) 79 (68) 107 (66) 167 (25) 166 (25) 234 (6)		
7	2025	++	Isomer of 19	79 (100) 137 (100) 138 (96) 107 (81) 139 (54) 179 (15) 193 (8)		
8	2031	++	Chloro-hydrocarbon	41 (100) 79 (33) 137 (26) 138 (26) 107 (24) 143 (20) 89 (17) 159 (1)		
9	2039	++	?	83 (100) 55 (49) 134 (36) 79 (31) 164 (18) 232 (4) 204 (2) 205 (1) 235 (1)		
10	2121	++	?	156 (100) 58 (98) 212 (25) 84 (17) 98 (8) 213 (4)		
11	2320	++	C ₂ -24 Alkane	41 (100) 57 (34) 71 (22) 85 (16) 99 (5)	Heptadecane, 9-octyl	619
12	2713	++	?	56 (100) 84 (16) 212 (29) 240 (7) 241 (5)		
13	2813	++	?	58 (100) 43 (45) 64 (14) 70 (8) 264 (38) 212 (43)		

TABLE A-158. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 58E

GC Peak No.	Retention Index	Amount, μg^b	tentative identification	Characteristic ions in Mass Spectrum	Most Reasonable Element Methyl Compound	K.I. J. 10 ²
1	902	***	Methoxybenzene	108(100)65(77)78(72)77(24)51(18)93(16)109(7)	Benzene Methoxy	551
2	990	***	Chlorophenol + Phenol	128(100)61(58)64(32)130(32)92(16)100(8)	Phenol, 2-Chloro-	324
3	1044	**	Methylphenol + Bromophenol	108(100)107(87)77(42)79(41)90(23)51(14)172(11)176(1)	Phenol, 2-Methyl-	659
4	1073	*	Benzoic Acid	105(100)77(74)136(32)51(28)	Benzoic Acid, Methyl Ester	333
5	1092	**	Methoxychlorobenzene	142(100)99(85)127(54)107(38)63(26)144(32)129(18)	Benzene, 1-Chloro-4-Methoxy-	584
6	1112	*	C $\geq$ 7 Fatty Acid	74(100)87(32)115(10)127(10)135(31)136(3)	Benzoic Acid, 5-Methyl-, Methyl Ester	327
7	1170	**	Dimethylphenol + C ₆ -Phenol	107(100)122(84)121(32)91(37)77(33)150(4)	Benzene, 1-Methoxy-2-Methyl-	445
8	1189	**	Methylbromophenol + Dichloromethoxy-	161(100)133(96)176(90)163(64)135(64)178(56)186(56)		
			benzene			
9	1220	*	Benzene, [(methoxymethoxy)methyl]	91(100)120(74)92(33)132(32)77(19)121(16)65(12)153(3)		
10	1232	*	C $\geq$ 9 Fatty Acid	74(100)87(40)143(11)		
11	1263	**	Dichlorophenol (methylated)	161(100)174(87)133(64)163(63)178(50)222(19)220(14)224(5)	Benzene, Dichloromethoxy-	399
12	1273	*	Hydroxymethylbenzoic Acid	106(100)134(95)166(48)77(41)78(31)105(37)135(36)211(3)	Benzoic Acid, 2-Hydroxy-3-Methyl, Methyl Ester	534
13	1282	*	C ₆ -alkylphenol	135(100)107(43)150(16)95(12)91(10)77(9)131(10)	Phenol, 4-[(1,1-Dimethyl Ethyl)]-	685
14	1309	*	C $\geq$ 10 Fatty Acid + Trichlorophenol	Mixed Spectrum		
15	1338	*	Bromophenol + ?	172(100)174(98)107(70)65(53)77(43)150(39)93(23)		
16	1357	*	Chloroalkylphenol + ?	91(100)120(50)163(40)207(9)222(9)205(6)220(6)		
17	1434	*	Chlorobromo-Subst. -Phenol	241(100)236(83)239(67)213(59)184(57)243(50)255(53)258(40)		
18	1499	*	Dimethoxybenzaldehyde	164(100)165(60)95(44)151(15)167(10)	Benzaldehyde, 3,4-Dimethoxy	553
19	1794	*	Benzene, 1-Methoxy-2-[(Methoxyphenyl)methyl]	228(100)91(98)107(97)197(76)181(64)132(57)229(15)	Benzene, 1-Methoxy-2-[(4-Methoxyphenyl)methyl]	346
20	1825	***	?	108(100)214(70)181(43)107(36)152(35)153(25)215(10)		
21	1856	**	C $\geq$ 16 Fatty Acid	74(100)87(82)143(23)227(6)270(2)228(2)	Hexadecanoic Acid, Methyl Ester	443
22	1896	**	Resin or Terner of #20 ?	108(100)121(24)152(22)214(56)197(17)224(8)		
23	1974	***	?	214(100)108(84)183(63)121(33)77(32)213(45)215(16)		
24	2048	***	Phenol, 2-[(4-Hydroxyphenyl)methyl]-	209(100)94(99)107(97)77(54)152(40)181(37)199(26)201(18)	Phenol, 2-[(4-Hydroxyphenyl)methyl]-	548
25	2113	*	C $\geq$ 18 Fatty Acid	74(100)87(86)143(20)298(2)		
26	2113	*	Terner of #24	107(100)200(75)199(45)	Phenol, 2[(4-Hydroxyphenyl)methyl]-	537

TABLE A-158. (Continued)

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	- Mass Resolvable Elements Match Compound	E.I. # 100
27	2304	ee	Octahydro C ₅ Alkylphenanthrene	239(100)240(21)197(18)299(12)314(6)355(3)	1-Phenanthrene Carboxylic Acid, 1,2,3,4,	556
			Carboxylic Acid N.E.		4a,9,10,10a-Octahydro-1,4a-Dimethyl-7-	
					(1-Methyl Ethyl)-Methyl Ester	
28	2396	e	Isomer of #27	237(100)238(20)312(10)397(8)313(2)		
29	2784	ee	?	121(100)107(18)91(24)227(25)228(13)334(22)335(6)		
30	2799	eee	Isomer of #29	107(100)213(41)91(34)121(23)226(10)334(18)335(5)		

TABLE A-159. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 59VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.15	10-100	Acetone	63(100)58(25)
3	.15	<1	Diethyl ether	45(100)59(98)74(51)
4	.16	1-10	Dichloromethane	49(100)84(37)
5	.19	1-10	Dichloroethane	63(100)65(30)83(15)98(6)100(4)
6	.22	<1	Chloroform	49(100)83(55)85(42)130(31)28(27)132(10)
7	.26	1-10	1,1,1-Trichloroethane	97(100)61(72)99(67)117,119(10)
8	.28	<1	Benzene	78(100)
9	.35	10-100	Trichloroethylene	95(100)132(70)128(68)97(61)
10	.45	<1	C ₇ H ₈ Alkene	55(100)83(80)41(40)42(40)69,98(25)
11	.54	10-100	Toluene	91(100)92(40)
12	.97	-(8)	1,5.	75(100)77(33)

TABLE A-160. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 60VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Chemical Identification	Characteristic ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.15	70-80	Furan	38(100) 68(95) 43(25) 34(5)
3	.16	<100	Dichloromethane	69(100) 84(85) 51(67)
4	.18	1-10	Dichloroethylene	61(100) 96(92) 98(62) 100(12)
5	.20	80-100	Dichloroethylene	61(100) 96(88) 98(52) 62(44)
6	.23	80-100	Chloroform	83(100) 85(90) 47(52)
7	.24	200-300	Tetrahydrofuran	42(100) 72(32) 71(31)
8	.26	1-10	1,1,1-Trichloroethane	97(100) 61(65) 97(62) 117, 119(10)
9	.29	90-100	Benzene	78(100)
10	.37	100-150	Trichloroethylene	95(100) 130(78) 138(73) 97(61)
11	.55	50-60	Toluene	91(100) 92(60)
12	.58	1-10	Dibromochloromethane	129(100) 127(80) 79, 81(29)
13	.68	50-70	Tetrachloroethane	166(100) 129(93) 131(88) 164(80) 94(58) 47(48)
14	.80	60-80	Chlorobenzene	112(100) 77(75)
15	.86	1-10	m-Chlorodinitrofluoride	180(100) 145(82) 75(70) 161(68) 50(62)
16	.88	1-10	C ₂ Alkyl benzene	91(100) 106(30)
17	.91	10-20	C ₂ Alkyl benzene	91(100) 106(42)
18	.98	10-20	O-xylene	91(100) 106(45)
19	.99	1-10	1,1,2,2-Tetrachloroethane	83(100) 85(67) 90, 61, 95(15) 131, 133(5) 166, 168(2)
20	1.00	-(8)	1,5.	75(100) 77(33)
21	1.08	1-10	C ₃ Alkyl benzene	105(100) 120(26)
22	1.13	10-20	C ₃ Alkyl benzene	91(100) 120(30)
23	1.14	<10	C ₃ Alkyl benzene + ?	91(100) 121(28) 63(16) 120(12) 123(11)
24	1.16	1-10	C ₃ Alkyl benzene	91(100) 120(20)
25	1.18	10-20	C ₃ Alkyl benzene	105(100) 120(30)
26	1.19	<10	C ₃ Alkyl benzene	105(100) 120(25)
27	1.20	1-10	C ₃ Alkyl benzene	105(100) 120(40)
28	1.22	1-10	C ₃ Alkyl benzene	105(100) 120(30)
29	1.26	10-20	C ₃ Alkyl benzene	105(100) 120(40) + small dichlorobenzene -- 1 ppb
30	1.27	1-10	Dichlorobenzene	166(100) 148(65) 111(50) 75(48)

TABLE A-161. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 60VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.03	500-1000	Acetone	43(100)88(100) 55(4)
2	0.04	40-50	Dichloromethane	49(100)84(55)
3	0.09	1-10	Methyl ethyl ketone	43(100)72(18)57(5)
4	0.10	10-20	Dichloroethylene	61(100)96(60)98(38)
5	0.11	60-70	Chloroform	83(100)85(63)
6	0.13	10-20	Tetrahydrofuran	43(100)41(52)72(28)71(27)
7	0.15	1-10	1,1,1-Trichloroethane	97(100)99(66)81(55)117,119(12)
8	0.17	10-20	Benzene	78(100)
9	0.18	1-10	Carbon tetrachloride	117(100)119(95)47(47)82(37)
10	0.22	1-10	2-Pentanone	43(100)86(10)58(6)71(5)
11	0.25	30-40	Trichloroethylene	95(100)130(84)132(82)97(63)
12	0.29	~1	Benzotrifluoride	146(100)91(62)127(58)141(52)
13	0.47	90-100	Toluene	91(100)92(60)
14	0.62	70-80	1,1,2,2-Tetrachloroethane	146(100)126(90)131(87)164(78)
15	0.76	10-20	Chlorobenzene	112(100)77(72)114(33)
16	0.85	~1	Ethyl benzene	91(100)106(33)
17	0.89	1-10	m- + p-Xylene	91(100)106(47)
18	0.97	1-10	o-Xylene	91(100)106(45)
19	1.00	~(8)	1,5-	75(100)77(33)
20	1.09	<1	C ₃ Alkyl benzene	105(100)120(25)
21	1.16	20-30	C ₃ Alkyl benzene + ?	91(100)121(30)89(17)63(16)123(11)120(9)
22	1.18	1-10	C ₃ Alkyl benzene + ?	91(100)121(26)63(15)65(10)89(9)120(9)123(8)
23	1.21	1-10	C ₃ Alkyl benzene	105(100)120(25)
24	1.22	1-10	C ₃ Alkyl benzene	105(100)120(22)
25	1.24	~1	C ₃ Alkyl benzene	105(100)120(42)
26	1.26	~1	C ₃ Alkyl benzene	105(100)120(25)
27	1.30	1-10	C ₃ Alkyl benzene	105(100)120(40)
28	--	1-10	Dichlorobenzene	146(100)148(65)75(57)111(52)
29	--	1-10	Dichlorobenzene	146(100)75(95)111(48)150(71)148(60)

TABLE A-162. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 601

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Textual Identification	Characteristic ions in Mass Spectrum	Most Plausible Chemical Name	E.I. $\times 10^3$
1	834	*	Tetrachloroethene	139(100)131(95)166(92)166(75)168(44)170(10)	Benzene, tetrachloro	548
2	849	**	Chlorobenzene	112(100)113(98)116(77)77(97)51(97)		
3	854	**	?	57(99)83(98)69(81)86(77)97(25)180(5)182(1)		
4	873	*	Ethylbenzene	91(100)106(82)92(75)77(35)51(46)	Benzene, 1,2-dimethyl	495
5	870	**	Ethylbenzene	92(100)91(95)106(86)105(39)51(40)77(37)25(25)65(26)	Benzene, 1,2-dimethyl	439
6	883	**	Tetrachloroethane	83(100)86(98)131(22)133(20)168(11)166(9)170(5)		
7	888	*	Butoxyethanol	57(100)45(67)41(53)87(10)75(10)100(2)	Ethanol, 1,2-bisoxo	848
8	910	*	C ₃ -Alkylbenzene	105(100)77(25)51(23)120(19)	Benzene, 1-methyl ethyl	712
9	930	**	Chloromethylbenzene	91(100)92(60)126(47)89(36)63(33)128(14)	Benzene (chloromethyl)	305
10	935	**	Chloromethylbenzene + C ₃ -Alkylbenzene	91(100)92(60)126(47)89(36)63(33)128(14)	Benzene (chloromethyl)	405
11	944	**	C ₃ -Alkylbenzene	105(100)120(58)77(43)79(35)91(30)51(25)65(20)	Benzene, 1-ethyl-2-methyl	542
12	960	**	C ₃ -Alkylbenzene	105(100)120(58)77(43)79(35)91(30)51(25)65(20)	Benzene (1-methyl ethyl)	395
13	976	**	C ₃ -Alkylbenzene	105(100)120(58)77(43)79(35)91(30)51(25)65(20)	Benzene (1,2,4-trimethyl)	562
14	985	**	1,3-Dichlorobenzene	75(100)111(99)146(98)146(97)50(75)113(31)130(15)	Benzene (1,4-dichloro)	430
15	1000	**	Decane	57(100)71(49)85(26)99(5)96(4)142(2)	Decane	502
16	1007	**	1,4-Dichlorobenzene	148(100)146(95)111(98)75(98)50(65)113(23)150(16)	Benzene, 1,4-dichloro	400
17	1022	**	Dichlorocyclohexane + C ₃ -Alkylbenzene	80(100)81(99)82(91)77(98)105(96)51(61)120(15)152(11)154(0.4)	Cyclohexane, 1,3-dichloro	237
18	1068	**	C ₆ -Alkylbenzene + ?	58(100)82(97)81(83)95(76)132(7)134(7)180(1.4)78(1.3)		
19	1099	**	Undecane + ?	57(100)71(96)85(50)156(3)		
20	1110	**	Bromochlorocyclohexane	82(100)81(99)79(63)53(38)117(16)119(6)		
21	1126	**	C ₂ -11 Alkane	57(100)43(59)71(50)85(16)117(16)123(7)184(0.3)186(0.3)		
22	1146	**	1,2,4-Trichlorobenzene	180(100)74(71)109(52)145(45)147(28)111(17)182(95)184(29)	Benzene, 1,2,3-trichloro	494
23	1151	**	Naphthalene	128(100)51(29)84(19)43(18)119(15)102(14)127(14)129(11)	Naphthalene	485
24	1178	**	C ₂ -11 Alkane	57(100)71(53)85(27)120(4)140(2)141(1.7)	Decane	648
25	1200	**	Dodecane + ?	58(100)71(97)85(56)98(8)99(7)170(0.7)	Dodecane	321
26	1228	**	C ₆ -Alkylbromobenzene	119(100)198(20)200(20)91(40)77(20)	Benzene, 2-bromo-1,3,5-trimethyl	546
27	1453	**	?	57(100)55(31)165(19)137(12)180(8)179(3)		
28	1554	**	C ₂ -15 Alkane + ?	76(100)56(97)85(95)100(56)145(4)143(2)147(2)175(1)		
29	1989	**	C ₂ -19 Alkane + ?	60(100)73(98)57(86)55(60)129(25)256(0.5)		
30	2000	**	Fluorene	53(100)40(46)52(46)55(40)73(37)102(26)756(0.4)		

TABLE A-162. (Continued)

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Responsible Element(s) in Compound	EL, $\times 10^3$
31	2035	oo	Pyrene + ?	202 (100) 101 (53) 57 (39) 88 (32) 71 (27) 200 (22) 203 (16) 201 (14)		
32	2050	oo	?	72 (100) 74 (83) 55 (61) 56 (60) 85 (60) 100 (32) 43 (5) 145 (4)		
33	2088	oo	Alkyl-alcohol, or alkane	57 (100) 70 (66) 83 (70) 97 (53) 111 (23) 125 (8) 208 (3)		
34	2099	oo	Hexacosane	71 (100) 85 (74) 57 (70) 99 (21) 113 (9) 127 (4) 218 (2)	Undecane, 2-methyl	438
35	2125	oo	?	58 (100) 184 (47) 43 (45) 44 (42) 71 (13) 84 (10) 185 (7)		
36	2150	oo	C > 21 alkane + ?	60 (100) 73 (94) 55 (82) 57 (77) 83 (50) 129 (36) 97 (30) 165 (8) 284 (1)		

TABLE A-164. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 60E

GC Peak No.	Retention Index	Amount, mg/l	Definitive Identification	Characteristic ions in Mass Spectrum	Most Reasonable Chemical Name	Ref. # 102
1	840	*	C ₂₂ 6 Fatty Acid	74(100)87(37)85(34)57(34)59(28)41(22)43(20)	Benzoic Acid, 3-Methyl-, Methyl Ester	536
2	899	**	Methoxybenzene	108(100)65(70)78(64)51(16)62(15)93(17)107(8)	Benzene, Methoxy-	517
3	912	**	C ₂₂ 6 Fatty Acid	74(100)87(41)43(42)59(30)99(22)101(10)104(2)	Pentanoic Acid, 3-Methyl-, Methyl Ester	420
4	975	**	Chlorophenol	128(100)130(76)65(80)64(58)66(34)82(38)100(18)73(17)	Phenol, 2-Chloro-	477
5	1013	***	Phenol	94(100)66(83)45(40)55(11)50(10)95(11)	Phenol	468
6	1031	*	C ₂₂ 7 Fatty Acid	87(100)102(65)57(27)41(26)115(15)130(12)128(11)	Heptanoic Acid, 2-Ethyl-, Methyl Ester	342
7	1031	*	Chloromethylphenol + 7	107(100)108(48)77(48)79(32)51(20)142(30)144(10)		
8	1043	**	Methylphenol + 9	108(100)107(49)77(49)79(49)90(23)51(20)172(20)174(20)	Phenol, 2-Methyl-	316
9	1040	*	Benzoic Acid	105(100)77(96)51(36)136(30)	Benzoic Acid	546
10	1089	***	Chloromethoxybenzene	145(100)99(83)127(55)107(47)144(32)77(30)63(26)129(18)	Benzene, 1-Chloro-4-Methoxy-	395
11	1090	**	C ₂₂ 7 Fatty Acid + 7	74(100)87(52)55(26)59(21)127(14)129(6)		333
12	1169	**	Dichlorophenol (methylated)	161(100)133(96)176(90)143(64)135(60)178(46)180(9)	Hexanoic Acid, 5-Methyl-, Methyl Ester	555
13	1185	*	Thienopyridine C ₁₀ H ₈ N ₂	135(100)108(36)69(21)82(12)136(8)	Benzoic Acid, 2-(Methylthio)-	606
14	1190	*	C ₂₂ 8 Fatty Acid	74(100)87(55)143(10)		
15	1204	**	Chlorobenzoic Acid	139(100)111(41)75(37)50(12)113(14)141(32)170(27)172(9)	Benzoic Acid, 3-Chloro, Methyl Ester	739
16	1210	**	Dichlorophenol (methylated) + 7	128(100)130(32)45(42)100(22)142(17)143(6)176(11)178(7)		
17	1224	**	Dichlorophenol (methylated)	161(100)176(86)133(85)163(64)135(54)178(32)	Benzene, Dichloromethyl-	540
18	1300	**	Trichlorophenol (methylated)	195(100)197(89)199(30)167(67)169(64)210(32)212(48)216(15)	Benzene, 1,2,4-Trichloro-5-Methoxy-	606
19	1333	**	Methoxy-1,2-Benzisothiazole	165(100)136(69)150(64)106(40)122(32)164(46)166(11)		417
20	1371	*	Chlorophenylmethanol	128(100)130(34)172(18)174(6)	Ethanol, 2-(4-Chlorophenyl)-	516
21	1391	*	Dichlorobenzoic Acid	173(100)135(66)145(26)147(18)206(18)208(12)	Benzoic Acid, 3,4-Dichloro-	701
22	1419	*	Dimethyl-1,2-Benzisothiazole	177(100)149(28)91(18)178(12)182(11)	1,2-Benzisothiazol-2-one, 5-(1,1-Dimethyl)-	289
23	1509	**	Dodecanoic Acid	74(100)87(74)55(29)143(14)183(5)185(3)216(2)	Dodecanoic Acid, Methyl Ester	436
24	1523	**	Methoxy-1,2-Benzisothiazole	136(100)69(14)122(12)96(8)95(7)137(10)165(65)66(6)	1,2-Benzisothiazole, 3-Methoxy-	218
25	1551	**	Methylthiobenzenethiazole	181(100)144(77)108(36)89(18)136(20)135(16)180(26)182(12)	Benzenethiazole, 2-(Methylthio)-	712
26	1692	*	Subst. -Benzisothiazole	151(100)123(73)96(35)195(20) Weak Spectra		
27	1708	*	Tetradecanoic Acid	74(100)87(75)55(31)143(20)199(10)211(3)213(1)	Tetradecanoic Acid, Methyl Ester	382
28	1804	*	C ₂₂ 13 Fatty Acid + 7	74(56)87(38)		389
29	1983	*	Subst. -Benzisothiazole	135(100)136(40)168(11)108(25)90(15)	Nonanoic Acid, Methyl Ester	504
30	2080	*	C ₂₂ 17 Fatty Acid	55(100)41(92)69(40)74(37)87(40)	11-Pentadecanoic Acid, Methyl Ester	416

TABLE A-164. (Continued)

GC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biomass Match Compound	R.I. # 103
31	2110	*	Octadecanoic Acid	74(100)87(76)43(43)35(34)143(24)199(10)	Nonacosanoic Acid, Methyl Ester	658

TABLE A-165. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 60E

GC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biomass Match Compound	R.I. # 103
1	952	**	Methylpyridine	93(100)46(33)65(17)92(12)84(7)	Pyridine, 3-Methyl	515
2	1044	***	Methylacetylene	106(100)107(72)77(17)79(13)89(2)51(7)	Benzenamine 4-Methyl	693
3	1083	**	7 H ₂ 126	41(100)40(80)126(80)43(77)67(52)88(49)86(28)125(10)127(6)	4(1H)-Pyridine 2,6-Diamine	
4	1137	**	Diamethylacetylene	121(100)120(67)106(95)77(22)91(16)103(10)		
5	1143	**	C ₃ -Alkylpyridine	121(100)120(92)106(92)77(21)91(16)	Pyridine, 3-Ethyl-5-Methyl	438
6	1169	*	C ₃ -Alkylpyridine	121(100)106(92)120(75)77(21)91(16)65(8)	Pyridine, 3-Ethyl-5-Methyl	389
7	1188	*	C ₃ -Alkylpyridine	106(100)121(91)120(55)77(20)91(15)107(12)65(10)	Pyridine, 3-Ethyl-4-Methyl	423

TABLE A-166. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 61VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.11		Air	44 (100)
2	.13	< 1	Butane	41 (100) 39 (50) 56 (40)
3	.15	1-10	Acetone	43 (100) 58 (22)
4	.16	1-10	Diethylether	45 (100) 59 (97) 74 (47)
5	.16	1-10	Dichloromethane	49 (100) 84 (35) 51 (33)
6	.17	< 1	Carbon disulfide	76 (100) 44 (12) 78 (8)
7	.25	< 1	Tetrahydrofuran	42 (100) 41 (90) 55 (55) 30 (52) 71 (28) 72 (27)
8	.26	< 1	1,1,1-Trichloroethane	97 (100) 61 (66) 99 (67) 119 (18) 117 (17)
9	.28	< 1	Benzene	78 (100)
10	.34	< 1	Dichloropropane	63 (100) 62 (70) 41 (52) 39 (40) 65 (32) 76 (25)
11	.36	< 1	Trichloroethylene	95 (100) 132, 99 (67) 130 (62) 60 (53)
12	.55	1-10	Toluene	91 (100) 92 (60)
13	1.00	-(8)	I.S.	75 (100) 77 (33)

TABLE A-167. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 61VE

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	---	Air	44(100)
2	.15	1-10	Acetone	43(100) 58(28)
3	.16	<10	Diethyl ether	45(100) 59(90) 74(40)
4	.16	1-10	Dichloromethane	49(100) 84(50)
5	.22	<1	Chloroform + I.S.	83(100) 49(95) 85(68) 130(28) 128(25) 47(28)
6	.24	1-10	Tetrahydrofuran	42(100) 41(55) 71(27) 72(26)
7	.26	<1	1,1,1-Trichloroethane	97(100) 99(66) 117(12) 119(13)
8	.28	<1	Benzene	Benzene
9	.30	1-10	Cyclohexane	56(100) 41(65) 84(60) 69(27)
10	.34	<1	Dichloropropane	63(100) 62(71) 41(50) 39(37) 65(31) 76(25)
11	.61	<1	Dibromomethane	107(100) 109(92)
12	.80	<1	Chlorobenzene	112(100) 77(97) 114(30)
13	1.00	-(8)	I.S.	75(100) 77(33)
14	1.09	<1	Unknown hydrocarbon	109(100) 95(90) 67(43) 81(40) 123(17)
15	1.12	<1	$\text{C}_{10}\text{H}_{20}\text{O}$	55(100) 69(88) 83(82) 41(78) 125(30)
16	1.15	1-10	Unknown hydrocarbon	109(100) 81(94) 67(40) 41(38) 95(22) 123(18)
17	1.18	1-10	Unknown hydrocarbon	81(100) 109(38) 41(35) 55(32) 67(27) 138(6)

TABLE A-168. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 62VI

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.15	1-10	Acetone	43(100)58(32)
3	.16	<1	Dichloroethylene	61(100)96(50)98(30)
4	.16	1-10	Dichloromethane	49(100)84(67)
5	.16	$\sim$ 1	Carbon disulfide	76(100)44(18)78(6)
6	.22	1-10	Chloroform	83(100)85(67)
7	.24	<1	Tetrahydrofuran + Chlorobutane	55(100)41(81)39(55)42(45)54(25)71(18)72(17)90(15)92(5)
8	.26	<1	1,1,1-Trichloroethane	97(100)99(67)61(62)119(12)117(10)
9	.28	$\sim$ 1	Benzene	78(100)
10	.33	<1	Dichloropropane	63(100)62(72)41(45)39(38)65(32)76(25)
11	.35	<1	Trichloroethylene	95(100)132(67)97(63)130(60)
12	.54	1-10	Toluene	91(100)92(55)
13	.67	<1	1,1,2,2-Tetrachloroethane	129(100)131(95)166(92)164(80)
14	.79	<1	Chlorobenzene	112(100)77(90)50.51(38)114(33)
15	1.00	-(8)	I.S.	75(100)77(33)

TABLE A-169. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 62VE

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.10	--	Air	44(100)
2	.11	20-40	Vinyl Fluoride (T)	46(100)45(99)
3	.12	40-60	Ethyl Chloride	64(100)49(82)66(70)
4	.14	60	Diethyl ether	45, 59, 74(100) (Sat'd)
5	.15	30-40	Dichloroethane (T)	49(100) no 84, 86
6	.16	~ 1	Chloropropane (T)	42(100)41(27)59(8)63(5)78(2)
7	.19	~ 10	Methoxy trimethyl silane	89(100)59(90)
8	.20	1-10	Unknown	45(100)43(80)41(30)57(20)87(15)133(2)
9	.22	100-1000	Unknown oxygen-containing compound	75(100)43(400)43(55)47(40)59(16)76(15)87(12)
10	.25	1-10	Dichloroethane	62(100)49(42)64(32)98(8)
11	.26	80-100	1,1,1-Trichloroethane	97(100)99(60)61(60)63(20)119(10)
12	.40	--	Silicone	147(100)73(25)
13	.51	~ 10	2-Ethyl-1,3-Dioxolane (T)	73(100)45(50)57(12)101(3)
14	.55	~ 1	Toluene	91(100)92(55)
15	.69	1-10	1,1,2,2-Tetrachloroethane	166, 129(100)131(95)164(80)
16	1.00	-(8)	I.S.	75(100)77(33)

TABLE A-170. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 62E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Ident. Reference Compound	E.I. $\times 10^3$
1	832	o	C ₂ & 6 Fatty acid	65(100) 87(72) 43(67) 55(36) 88(14) 99(7)		
2	836	o	C ₂ & 6 Fatty acid	74(100) 42(52) 67(36) 55(27) 99(17) 101(8)	Pentanoic acid, 3-methyl methyl ester	510
3	840	oo	Carbital	45(100) 59(34) 72(74) 104(23) 103(2)	Ethane, 1,1'-oxy bis(2-ethoxy)-	630
4	885	o	C ₂ & 6 Fatty acid	87(100) 102(66) 57(42) 115(12) 130(9) 129(8)	Septanoic acid, 2-ethyl, methyl ester	450
5	913	o	Methylphenol	104(100) 107(89) 79(69) 77(48) 51(22) 90(24) 109(8)	Phenol, 2-methyl-	546
6	1046	oo	?	57(100) 59(40) 75(26) 117(21) 85(18) 121(5)		
7	1278	oo	Ethane, 1,1'-oxybis(2-ethoxy)	45(100) 59(96) 73(40) 72(38) 117(40) 147(1)		
8	1372	o	Polypropylene glycol methyl ether	59(100) 41(80) 117(62) 45(56) 73(40) 146(6)		
9	1418	o	Ethane, 1,2-bis(2-ethoxyethoxy)ethoxy	59(100) 45(94) 117(70) 73(48) 147(2) 148(1) 181(1)		
10	1435	o	11,11-dimethyl benzenesulfonamide	91(100) 65(32) 155(16) 121(12) 185(14) 186(1)	benzenesulfonamide, 11,11-dimethyl	645
11	1722	oo	Polypropylene glycol methyl ether	59(100) 117(88) 41(72) 73(40) 131(2) 147(1)		
12	1804	o	C ₂ & 15 Fatty acid	55(100) 74(60) 87(41) 236(2) 237(1)	10-undecanoic Acid	583
13	1983	oo	Polypropylene glycol methyl ether	59(100) 45(81) 117(88) 73(32) 87(27) 103(12) 131(4)		
14	2109	o	Polypropylene glycol methyl ether	59(100) 41(64) 45(43) 103(27) 73(23) 87(22)		
15	2130	o	Polypropylene glycol methyl ether	45(100) 41(43) 69(40) 87(25) 133(10) 73(25)		
16	2249	oo	Polypropylene glycol methyl ether	59(100) 45(64) 41(58) 117(98) 129(6) 133(4) 131(3) 181(3)		
17	2513	oo	Polypropylene glycol methyl ether	117(100) 59(83) 45(43) 73(32) 129(6) 133(6) 16(5) 175(1)		
18	2765	oo	Polypropylene glycol methyl ether	117(100) 59(87) 45(40) 73(36) 133(7) 129(6) 161(4) 175(0.7)		

TABLE A-171. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 62E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Ident. Reference Compound	E.I. $\times 10^3$
1	845	oo	? 1H 149	149(100) 133(89) 150(15) 134(12) 75(11) 115(7) 67(4)		
2	933	oo	8-licone? 1H 205	59(100) 43(74) 85(18) 103(11) 205(16) 206(3)		
3	955	ooo	11-butoxyl-1-butanamine	44(100) 86(96) 41(21) 57(18) 129(13)	1-butanamine, 11-butoxyl-	449
4	960	o	11-butoxyl, 11-butoxyl-1-butanamine	58(100) 100(76) 44(49) 86(26) 143(9) 129(3)	1-butanamine, 11-butoxyl-11-butoxyl-	542
5	982	o	8-licone? 1H 223	207(100) 208(21) 91(18) 273(16) 133(13) 75(8)		
6	1087	oo	?	59(100) 41(55) 45(49) 73(33) 103(23)		
7	1332	oo	?	97(100) 139(80) 142(32) 83(40) 100(32) 42(26) 182(3)		

TABLE A-172. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 63VI

GC Peak No.	Relative Retention Time	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.16	1-10	Acetone	43(100)58(20)
3	.16	1-10	$\text{C}_2\text{H}_6\text{S}$, e.g. Dimethyl sulfide	62(100)47(93)55(55)46(40)61(37)
4	.17	<10	Dichloromethane	49(100)84(35)
5	.22	1-10	Chloroform	83(100)85(67)
6	.25	<1	Tetrahydrofuran + 2 Chloro-2-butenes	42(100)41(96)55(75)39(55)75(32)71(30)90(15)92(5)
7	.27	<1	1,1,1-Trichloroethane	97(100)99(67)61(50)119(15)117(14)
8	.29	<1	Benzene	78(100)
9	.34	<1	Dichloropropane	63(100)62(68)41(52)39(40)76(18)
10	.37	<1	Trichloroethylene	95(100)97.132(65)130(57)
11	.41	<1	Methylmethacrylate (T)	41(100)69(60)39(40)99(15)100(14)
12	.80	<1	Chlorobenzene	112(100)77(80)114(33)
13	1.00	-(8)	I.S.	75(100)77(33)
14	1.17	<1	Unknown	55(100)91(40)93(20)

TABLE A-173. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 63VE

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.06	--	Air	44(100)
2	.10	1-10	Acetone	43(100)44(40)58(25)
3	.11	>1000	Dimethyl sulfide	45,46,47,61,62(100)
4	.45	1-10	Dimethyl disulfide	94(100)45(93)79(62)46(50)
5	1.00	(8)	I.S.	75(100)77(33)

TABLE A-174. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 63E

GC Peak No.	Retention Index	Amount, $\mu\text{g/l}$	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Chemical Match Compound	R.I. ± 10
1	1005	*	Chlorobenzene	112(100)77(82)51(30)114(32)50(27)	Benzene, chloro	432
2	1509	*	Methyl 4-chlorophenyl sulfone	139(100)111(92)75(56)141(32)113(30)190(4)182(1)		
3	1853	*	Benzene, 1,1'-sulfonylbis-	125(100)77(49)51(44)97(20)218(5)		
4	1917	*	Dibutyl phthalate	149(100)41(12)150(6)205(1)223(1)	Benzene, 1,1'-sulfonylbis- 1,2-benzenedicarboxylic acid, butyl-2-methyl propyl ester	417 630
5	2174	***	Benzene, 1,1'-sulfonylbis(4-chloro)-	159(100)75(74)111(52)161(36)286(8)288(5)290(1)	Benzene, 1,1'-sulfonylbis(4-chloro)-	338
6	2138	***	Benzene, 1,1'-sulfonylbis(4-chloro)	75(100)159(99)111(90)50(64)161(65)286(16)288(11)290(2)	"	335